

10/519,163

(FILE 'HOME' ENTERED AT 18:29:10 ON 16 MAR 2006)

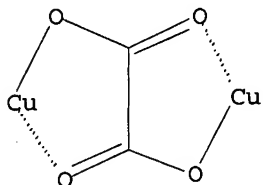
FILE 'REGISTRY' ENTERED AT 18:29:35 ON 16 MAR 2006

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 18:29:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 83 TO ITERATE

100.0% PROCESSED 83 ITERATIONS

21 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1114 TO 2206

PROJECTED ANSWERS: 146 TO 694

L2 21 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 18:29:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1553 TO ITERATE

100.0% PROCESSED 1553 ITERATIONS

337 ANSWERS

SEARCH TIME: 00.00.01

L3 337 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 18:30:08 ON 16 MAR 2006

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FILE COVERS 1907 - 16 Mar 2006 VOL 144 ISS 12

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=> s 13

L4 138 L3

=> s 14 and py<2002

21808282 PY<2002

L5 89 L4 AND PY<2002

=> d 1-89 bib abs

L5 ANSWER 1 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:560392 CAPLUS

DN 135:297586

TI A novel salt formed by mixed-valence vanadium(IV,V) [(VO)2O(bpy)2(C2O4)2] anions and ferromagnetic [Cu2(bpy)4(C2O4)] cations: structure, spectroscopic characterization and magnetic properties

AU Costisor, Otilia; Brezeanu, Maria; Journaux, Yves; Mereiter, Kurt; Weinberger, Peter; Linert, Wolfgang

CS Inorganic Chemistry Laboratory, Timisoara Branch, Romanian Academy of Sciences, Timisoara, 1900, Rom.

SO European Journal of Inorganic Chemistry (2001), (8), 2061-2066

CODEN: EJICFO; ISSN: 1434-1948

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 135:297586

AB The new heterometallic, mixed-valence compound [Cu2(bpy)4(C2O4)][(VO)2O(bpy)2(C2O4)2]·10H2O was synthesized, its crystal structure determined and its spectroscopic characterization accomplished by solid-state vibrational (far and mid FTIR) spectroscopy. The title compound crystallizes in the triclinic system, space group P<sub>h</sub>1<sub>h</sub>1 [a 13.488(5), b 14.160(6), c 15.829(9) Å, α 87.22(2), β 66.33(2), γ 64.49(2)°, Z = 1]. The compound consists of the cationic binuclear copper(II) complex [Cu2(bpy)4(C2O4)]<sup>2+</sup>, two anionic binuclear mixed valence vanadium(IV)-vanadium(V) complexes [(VO)2O(bpy)2(C2O4)2]<sup>-</sup>, and ten uncoordinated water mols. The copper atom exhibits a Jahn-Teller-distorted octahedral coordination. The vanadium atoms adopt a strongly distorted octahedral coordination and form a characteristic O:V-O-V:O moiety with a significantly bent V-O-V link. The temperature dependence of the magnetic susceptibilities was studied in the temperature range 2-300 K and explained in terms of the ferromagnetic interaction between CuII ions giving J = 22.7 yJ (1.14 cm<sup>-1</sup>) and g = 2.014.

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:557583 CAPLUS

DN 135:312648

TI Synthesis, crystal structure and magnetic properties of a new oxalato-bridged binuclear copper(II) complex with a tridentate Schiff base ligand

AU Bag, B.; Mondal, N.; Mitra, S.; Gramlich, V.; Ribas, J.; El Fallah, M. S.

CS Department of Chemistry, Jadavpur University, Calcutta, 700032, India

SO Polyhedron (2001), 20(17), 2113-2116

CODEN: PLYHDE; ISSN: 0277-5387

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 135:312648

AB A new oxalato-bridged binuclear Cu(II) complex, [{Cu(L)}2OX] (1; L = 2-N-(2'-pyridylimine)benzoic acid) was synthesized and characterized by ESR and IR spectra and variable temperature magnetic susceptibility measurements. The single crystal x-ray diffraction reveals that, both the Cu(II) ions have distorted square pyramidal geometry with the coordination of the tridentate Schiff base ligand and the oxalate group. The Cu(II)

centers are separated by 5.4 Å and antiferromagnetically coupled with a singlet-triplet separation of -12.4 cm<sup>-1</sup>.

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:476263 CAPLUS  
DN 135:160346  
TI An oxalato-bridged copper(II) complex  
AU Cheng, Jack; Liao, Fen Ling; Lu, Tian Huey; Mukherjee, Partha S.; Maji, Tapas K.; Chaudhuri, N. Ray  
CS Department of Physics, National Tsing Hua University, Hsinchu, 300, Taiwan  
SO Acta Crystallographica, Section E: Structure Reports Online (2001), E57(7), m263-m264  
CODEN: ACSEBH; ISSN: 1600-5368  
URL: <http://journals.iucr.org/e/issues/2001/07/00/bt6045/bt6045.pdf>  
PB International Union of Crystallography  
DT Journal; (online computer file)  
LA English  
AB Crystals of the title compound,  $\mu$ -oxalato-bis[(isocyanato-N)(tetramethylethylenediamine)copper(II)], are monoclinic, space group P2<sub>1</sub>/c, with a 7.4943(9), b 14.5660(17), c 10.8812(13) Å,  $\beta$  105.655(2)°; Z = 2, dc = 1.543; R = 0.039, R<sub>w</sub>(F<sub>2</sub>) = 0.090 for 2734 reflections. The CuII ions are five-coordinated. One CuII ion bridges to another centrosymmetry-related CuII ion through C2O4<sup>2-</sup>, forming a plane with an root-mean-square deviation of 0.059 Å. The O-Cu-O angle is 79.33(8)° and the Cu...Cu separation is 5.14 Å.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:428233 CAPLUS  
DN 135:220106  
TI One-dimensional oxalato-bridged copper(II) complex possessing two structurally different metallic centres  
AU Castillo, O.; Luque, A.; Lloret, F.; Roman, P.  
CS Departamento de Quimica Inorganica, Universidad del Pais Vasco, Bilbao, E-48080, Spain  
SO Inorganic Chemistry Communications (2001), 4(7), 350-353  
CODEN: ICCOFP; ISSN: 1387-7003  
PB Elsevier Science S.A.  
DT Journal  
LA English  
OS CASREACT 135:220106  
AB The crystal structure of the newly prepared oxalato-bridged copper(II) compound [Cu<sub>2</sub>( $\mu$ -ox)<sub>2</sub>(ampy)<sub>3</sub>]<sub>n</sub> (1, ox = oxalate dianion, ampy = 2-amino-3-methylpyridine) consists of infinite corrugated 1-dimensional chains in which two types of copper(II) centers, five- and six-coordinated, are bridged sequentially by asym. bis-bidentate oxalato ligands. Magnetic susceptibility measurements show the occurrence of a significant intrachain antiferromagnetic coupling (J = -22.9 cm<sup>-1</sup>).

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:397787 CAPLUS  
DN 135:297521  
TI Synthesis and crystal structure of oxalato-bridged dicopper(II) complex with reduced imino nitroxide radicals  
AU Li, L.; Liao, D.; Bai, L.; Jiang, Z.; Yan, S.  
CS Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China  
SO Journal of Molecular Structure (2001), 569(1-3), 179-183  
CODEN: JMOSB4; ISSN: 0022-2860  
PB Elsevier Science B.V.  
DT Journal  
LA English  
AB The new oxalato-bridged dicopper(II) complex [Cu<sub>2</sub>( $\mu$ -C<sub>2</sub>O<sub>4</sub>)(Him<sup>2-</sup>py)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>].CH<sub>3</sub>OH was synthesized and its crystal structure determined by x-ray

diffraction methods. The imino nitroxide 2-(2'-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-oxyl (i.m.2-py) is reduced in the reaction to yield 2-(2'-pyridyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazolyl-1-hydroxy (Him2-py). The structure consists of centrosym. [Cu<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(Him2-py)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>] and one solvent methanol mol. Each Cu(II) ion is in a distorted tetragonal pyramid environment with two nitrogen atoms from Him2-py and two oxygen atoms from the oxalate ion in the basal plane, and one oxygen atom from the nitrate group in the axial position.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:392580 CAPLUS  
DN 135:146271  
TI Synthesis and magnetic study of new μ-oxalato dinuclear copper (II) complexes  
AU Mukherjee, Partha Sarathi; Maji, Tapas Kumar; Koner, Subratanath; Rosair, Georgina; Chaudhuri, Nirmalendu Ray  
CS Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032, India  
SO Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (2001), 40A(5), 451-455  
CODEN: ICACEC; ISSN: 0376-4710  
PB National Institute of Science Communication, CSIR  
DT Journal  
LA English  
OS CASREACT 135:146271  
AB Three new μ-oxalato dinuclear Cu(II) complexes [L(H<sub>2</sub>O)CuOxCu(H<sub>2</sub>O)L](ClO<sub>4</sub>)<sub>2</sub> [L = 4-(2-aminoethyl)morpholine (aem), (1), 1-(2-aminoethyl)piperidine (ampp), (2) and 1-(2-aminoethyl)pyrrolidine (ampy), (3)] were synthesized and characterized by x-ray single crystal anal. (for 1), IR, thermal anal. and magnetic measurements. Low temperature magnetic measurements of these complexes show the existence of strong antiferromagnetic interaction between the Cu(II) ions.

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:314376 CAPLUS  
DN 135:146192  
TI A 1D coordination polymer of copper(II) with three different bridging anions: synthesis, crystal structure and magnetic behaviour  
AU Sarathi Mukherjee, Partha; Kumar Maji, Tapas; Mostafa, Golam; Hibbs, Wendy; Ray Chaudhuri, Nirmalendu  
CS Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700032, India  
SO New Journal of Chemistry (2001), 25(5), 760-763  
CODEN: NJCHE5; ISSN: 1144-0546  
PB Royal Society of Chemistry  
DT Journal  
LA English  
OS CASREACT 135:146192  
AB Reaction of Cu(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O with N,N'-dipropylethane-1,2-diamine (dpren, L), sodium oxalate and sodium azide in a 2:2:1:1 molar ratio results in a 1-dimensional coordination polymer [(μ-ClO<sub>4</sub>)<sub>1/2</sub>L(H<sub>2</sub>O)Cu(ox)-Cu(H<sub>2</sub>O)L(μ-N<sub>3</sub>)<sub>1/2</sub>]<sub>n</sub>(ClO<sub>4</sub>)<sub>n</sub>, bridged through alternate azide and perchlorate anions, which, on mutual interaction with neighboring 1-dimensional chains through H-bonding via interchain free perchlorate anions, produces a sheet-like structure. A low temperature magnetic measurement of the complex shows the existence of strong antiferromagnetic interactions between the copper(II) ions. Least-squares fitting of the exptl. magnetic susceptibility data using a modified Bleaney-Bowers equation for a dinuclear copper(II) system leads to the parameters J = -331.3 cm<sup>-1</sup> and g = 2.05. The complex also was characterized by x-ray single-crystal structure anal. and IR spectroscopy.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:255436 CAPLUS

DN 135:101425

TI One-dimensional oxalato-bridged copper(II) complexes with  
3-hydroxypyridine and 2-amino-4-methylpyridine

AU Castillo, O.; Luque, A.; Julve, M.; Lloret, F.; Roman, P.

CS Departamento de Quimica Inorganica, Universidad del Pais Vasco, Bilbao,  
E-48080, Spain

SO Inorganica Chimica Acta (2001), 315(1), 9-17

CODEN: ICHAA3; ISSN: 0020-1693

PB Elsevier Science S.A.

DT Journal

LA English

OS CASREACT 135:101425

AB Two new 1-dimensional oxalato-bridged Cu(II) compds. [Cu(ox)L2]n (1) and  
{[Cu2(ox)2L'3]·L'}n (2) [ox = oxalate dianion, L =  
3-hydroxypyridine (pyOH) and L' = 2-amino-4-methylpyridine (ampy)] were  
synthesized and characterized by FTIR spectroscopy, variable-temperature  
magnetic measurements and single-crystal x-ray diffraction. The crystal  
structure of 1 comprises chains of Cu atoms in which cis-[Cu(pyOH)2]2+  
units are sequentially bridged by asym. bis-bidentate oxalato ligands with  
an intrachain Cu-Cu separation of 5.548(1) Å. Each Cu atom is  
six-coordinated: four O atoms belonging to two bridging oxalato ligands  
and two N atoms from two 3-hydroxypyridine ligands build a distorted  
octahedral environment around the metal atom. As in 1, the structure of  
compound 2 is made up of chains of Cu atoms bridged sequentially by  
bis-bidentate oxalato ligands. Two types of Cu(II) ion, one being  
six-coordinated (Cu(1)) and the other five-coordinated (Cu(2)), alternate  
regularly within the chain. The environment around Cu(1) is elongated  
octahedral with two cis-coordinated pyridine-N and two O atoms from two  
oxalate ligands building the equatorial plane, the apical positions being  
filled by two oxalate-O atoms. The environment around Cu(2) is distorted  
square pyramidal with four oxalato-O atoms in the basal plane, and the  
pyridine N atom from one aromatic base in the apical position. Magnetic  
susceptibility data in the temperature range 2.0-300 K reveal regular  
ferromagnetic (J = +1.3 cm<sup>-1</sup>) and alternating antiferromagnetic (J = -66.6  
cm<sup>-1</sup>, αJ = -58.6 cm<sup>-1</sup>) chain behaviors for 1 and 2. The nature and  
magnitude of the magnetic coupling through the oxalato bridge in 1 and 2  
are analyzed and discussed in the light of the available structural data.

RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:149458 CAPLUS

DN 134:216474

TI Crystal structure of dibarium bis(nitrilotriacetato)(μ-  
oxalato)docuprate(II) octahydrate Ba2[Cu2(Nta)2(Oxal)]·8H2O

AU Polyakova, I. N.; Poznyak, A. L.; Sergienko, V. S.

CS Inst. Obshchei i Neorg. Khim. im. N. S. Kurnakova, RAN, Moscow, Russia

SO Zhurnal Neorganicheskoi Khimii (2000), 45(10), 1649-1651

CODEN: ZNOKAQ; ISSN: 0044-457X

PB MAIK Nauka/Interperiodica Publishing

DT Journal

LA Russian

AB The title compound was obtained from the reaction of BaHNta.1.5H2O and  
CuCO3.Cu(OH)2 in aqueous solution, and its crystal structure was determined by x-ray  
anal. Crystals are monoclinic, space group P21/c, with a 9.134(2), b  
8.811(2), c 18.013(4) Å, β 101.53(3)°; Z = 2, dc = 2.362;  
R = 0.0276, Rw = 0.0306 for 3588 reflections. Atomic coordinates are given.  
The structure consists of dimeric centrosym. anions [Cu2(Nta)2(oxal)]4-  
and hydrated Ba cations. The bridging oxalato connects the 2 Cu atoms and  
precludes formation of polymeric complexes. The Cu atom has distorted  
tetragonal bipyramidal coordination by a N and 3 O atoms of the  
tetradentate ligand Nta3- and 2 O atoms of the oxalato anion.

L5 ANSWER 10 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:909869 CAPLUS

DN 134:202064

TI Fixing Carbon Dioxide with Copper: Crystal Structure of  
 [LCu( $\mu$ -C2O4)CuL][Ph4B]2 (L = N,N',N''-Triallyl-1,4,7-triazacyclononane)  
 AU Farrugia, Louis J.; Lopinski, Stefan; Lovatt, Paul A.; Peacock, Robert D.  
 CS Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK  
 SO Inorganic Chemistry (2001), 40(3), 558-559  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 134:202064  
 AB The reaction of carbon dioxide with a solution of CuI, NaBPh4 and  
 N,N',N''-triallyl-1,4,7-triazacyclononane (L) resulted in the formation of  
 the oxalato bridged dinuclear copper(II) complex [LCu( $\mu$ -  
 C4O4)CuL](BPh4)2. The complex can be prepared in higher yields using CsHCO3  
 in place of CO2. The crystal structure of the complex was determined showing  
 square pyramidal geometries for the copper atoms with nitrogen atoms in  
 the axial positions. Variable temperature magnetic susceptibility measurements  
 show it to be antiferromagnetic ( $J = -274 \text{ cm}^{-1}$ ) as expected for this type  
 of structure.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2000:859408 CAPLUS  
 DN 134:78945  
 TI Crystal structure of bis(N,N,N',N'-tetramethylethylenediamine)-O,O'- $\mu$ -  
 O,O'-oxalato-dihydroxydicopper(II)  
 AU Hokelek, Tuncer; Unaleroglu, Canan; Mert, Yuksel  
 CS Department of Physics, Hacettepe University, Ankara, 06532, Turk.  
 SO Analytical Sciences (2000), 16(11), 1235-1236  
 CODEN: ANSCEN; ISSN: 0910-6340  
 PB Japan Society for Analytical Chemistry  
 DT Journal  
 LA English  
 AB The title compound was prepared from mixts. of L-ascorbic acid,  
 N,N,N',N'-tetramethylethylenediamine, and Cu methoxide in absolute methanol.  
 Crystals of the title compound are triclinic, space group P.hivin.1, with a  
 7.288(1), b 7.461(1), c 10.701(1) Å,  $\alpha$  69.65(1),  $\beta$   
 78.17(1),  $\gamma$  81.45(1)°; Z = 1, dc = 1.50; R = 0.024 Rw = 0.033  
 for 2044 reflections. Atomic coordinates are given. The compound consists of  
 symmetry related tetramethylethylenediamine ligands and hydroxy ions  
 bonded to Cu ions, linked by planar bridging oxalate ligands in trans  
 positions.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2000:830776 CAPLUS  
 DN 134:136890  
 TI Bonding Preferences of C2X4-Bridged Bimetallic Transition Metal Complexes  
 of Ti, Cu, and Ag  
 AU Mire, Lisa W.; Marynick, Dennis S.  
 CS Department of Chemistry and Biochemistry, University of Texas at  
 Arlington, Arlington, TX, 76051-0065, USA  
 SO Inorganic Chemistry (2000), 39(26), 5970-5975  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB The bonding preference of transition metal species of general formula  
 [(PH3)2M]2( $\mu$ -C2X4), where M = Cu or Ag and X = O, S, Se, or Te, and  
 (Cp2Ti)2( $\mu$ -C2X4), where X = S or Se, are explored using d. functional  
 theory. The relative energies of metal binding to the bridging ligand in  
 a dithiolene-like vs dithiocarbamate-like manner are evaluated. In all  
 cases, the most stable structure corresponds to dithiolene-like (or  
 side-side) bonding, consistent with the vast majority of these compds.  
 which have been exptl. characterized. However, for M = Ag and X = S, Se,  
 or Te, the two isomers are nearly degenerate.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:808141 CAPLUS  
DN 134:122781  
TI Excitation Energy Dedicated Molecular Orbitals. Method and Applications to  
Magnetic Systems  
AU Calzado, Carmen J.; Malrieu, Jean-Paul; Cabrero, Jesus; Caballol, Rosa  
CS Laboratoire de Physique Quantique IRSAMC, Universite Paul Sabatier,  
Toulouse, 31062, Fr.  
SO Journal of Physical Chemistry A (2000), 104(49), 11636-11643  
CODEN: JPCAFH; ISSN: 1089-5639  
PB American Chemical Society  
DT Journal  
LA English  
AB This paper proposes a general strategy to define MOs which are especially  
adapted to the calcn. of the energy difference between 2 states. These  
orbitals are eigenvectors of blocks of the difference between the d.  
matrixes relative of the 2 states. They may be used for rational  
enlargement of the active space in CASSCF calcns. or for truncations of  
the CI space. Several examples show the relevance of the method to  
identify the few MOs of a bridge between magnetic centers which play a  
role in the spin coupling mechanism.  
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:720743 CAPLUS  
DN 134:61825  
TI Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II)  
Dinuclear Complexes  
AU Cabrero, J.; Ben Amor, N.; de Graaf, C.; Illas, F.; Caballol, R.  
CS Departament de Quimica Fisica i Inorganica and Institut d'Estudis  
Avancats, Universitat Rovira i Virgili, Tarragona, 43005, Spain  
SO Journal of Physical Chemistry A (2000), 104(44), 9983-9989  
CODEN: JPCAFH; ISSN: 1089-5639  
PB American Chemical Society  
DT Journal  
LA English  
AB The structural dependence of the coupling constant in a series of  
[L3Cu( $\mu$ -C2O4)CuL3]2+ complexes was analyzed by means of ab initio  
difference-dedicated CI (DDCI2) calcns. on the model ( $\mu$ -  
oxalato)bis[triamminecopper(II)] cation, [(NH3)6Cu2( $\mu$ -C2O4)]2+, in  
which the nitrogen-coordinated ligands were substituted by NH3. Two types  
of geometrical structures were considered: three different C2h geometries  
and four crystallog. centrosym. geometries taken from [(Et5dien)2Cu2( $\mu$ -  
C2O4)](BPh4)2 and [(Et5dien)2Cu2( $\mu$ -C2O4)](PF6)2 (Et5dien =  
1,1,4,7,7-pentaethyldiethylenetriamine), [(tmen,2-MeIm)2Cu2( $\mu$ -  
C2O4)](PF6)2 (tmen = N,N,N',N'-tetramethylethylenediamine and 2-MeIm =  
2-methylimidazole), and [(dien)2Cu2( $\mu$ -C2O4)](ClO4)2 (dien =  
diethylenetriamine). The antiferromagnetic coupling is strongly  
underestimated when pure DDCI2 calcns. are performed, but when the CI  
space includes the relaxation of the oxalato-copper charge transfer,  
quant. agreement with the exptl. results is reached with an error smaller  
than 5 cm-1. The role of the external ligands in the model is also  
discussed by means of broken symmetry DFT calcns. At this level of  
theory, a very different influence of the ligands is predicted by  
different exchange-correlation functionals; therefore, the use of DFT to  
investigate this effect should be considered with caution.  
RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:472002 CAPLUS  
DN 133:159277  
TI Synthesis and magnetic properties of binuclear copper(II) complex with a  
bridging oxalate, Cu2(C15H26N2)2( $\mu$ -C2O4)(NO3)2  
AU Lee, Yong-Min; Jung, Hee-Cheul; Choi, Sung-Nak; Hur, Nam Hwi  
CS Department of Chemistry, Pusan National University, Pusan, 609-735, S.

Korea  
SO Journal of the Korean Chemical Society (2000), 44(2), 166-169  
CODEN: JKCSEZ; ISSN: 1017-2548  
PB Korean Chemical Society  
DT Journal  
LA English  
AB Reaction of copper(II) (-)-sparteine (L) dinitrato complex [Cu(L)(NO<sub>3</sub>)<sub>2</sub>] with sodium oxalate gave binuclear oxalate-bridged product Cu<sub>2</sub>(L)<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(NO<sub>3</sub>)<sub>2</sub> in 725 yield. The product was characterized by elemental anal., IR and FAB-mass spectral data. The ESR spectrum is consistent with the oxalate-bridged dimeric structure. The complex exhibits strong antiferromagnetic interaction with the maximal susceptibility at 150 K.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:458158 CAPLUS  
DN 133:144002  
TI Self-assembly, structures, and magnetic properties of ladder-like copper(II) coordination polymers  
AU Min, Kil Sik; Suh, Myunghyun Paik  
CS School of Chemistry and Center for Molecular Catalysis, Seoul National University, Seoul, 151-742, S. Korea  
SO Journal of Solid State Chemistry (2000), 152(1), 183-190  
CODEN: JSSCBI; ISSN: 0022-4596  
PB Academic Press  
DT Journal  
LA English  
AB Two novel ladder-like copper(II) compds., [Cu<sub>2</sub>(histamine)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(ClO<sub>4</sub>)<sub>2</sub>] (1) and [Cu<sub>2</sub>(histamine)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>(NO<sub>3</sub>)<sub>2</sub>] (2), were prepared. Compound 1 crystallizes in the triclinic space group P<sub>2</sub><sub>1</sub>/c, with a 7.450(4), b 7.519(7), c 9.646(5) Å, α 85.78(7), β 88.60(4), γ 76.78(7)°, and Z = 1 with R = 0.0789 (all data). In 1, the dinuclear units of [Cu<sub>2</sub>(histamine)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]<sub>2</sub><sup>+</sup> are linked together by the perchlorate anions to form a ladder-like chain. The chains interact each other by the π-π stacking interactions via the imidazole groups. Compound 2 crystallizes in the triclinic space group P<sub>2</sub><sub>1</sub>/c, with a 7.579(2), b 8.133(1), c 9.161(3) Å, α 77.06(2), β 89.23(2), γ 82.54(1)°, and Z = 1 with R = 0.0751 (all data). In 2, each dinuclear unit [Cu<sub>2</sub>(histamine)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]<sub>2</sub><sup>+</sup> is coordinated with a nitrate anion and a water mol., and they are held together by the hydrogen bonding interactions to form a ladder-like chain. The magnetic susceptibility data of 1 and 2 measured in 2-300 K provide the magnetic parameters, g = 2.08, J = -166 cm<sup>-1</sup>, J' = 6.46 cm<sup>-1</sup>, ρ = 0.0026, N<sub>A</sub> 155. + 10<sup>-6</sup> cm<sup>3</sup> mol<sup>-1</sup>, and R = 1.03 + 10<sup>-3</sup> (g = 2.05, J = -162 cm<sup>-1</sup>, J' = 10.5 cm<sup>-1</sup>, ρ = 0.0029, and R = 2.95 + 10<sup>-3</sup> with the fixed value of N<sub>A</sub> 120. + 10<sup>-6</sup> cm<sup>3</sup> mol<sup>-1</sup>) for 1 and g = 2.00, J = -158 cm<sup>-1</sup>, J' = 26.5 cm<sup>-1</sup>, ρ = 0.0020, N<sub>A</sub> 136. + 10<sup>-6</sup> cm<sup>3</sup> mol<sup>-1</sup>, and R = 7.31 + 10<sup>-4</sup> (g = 2.01, J = -157 cm<sup>-1</sup>, J' = 25.0 cm<sup>-1</sup>, ρ = 0.0021, and R = 1.32 + 10<sup>-3</sup> with the fixed value of N<sub>A</sub> 120. + 10<sup>-6</sup> cm<sup>3</sup> mol<sup>-1</sup>) for 2. These indicate that very strong antiferromagnetic interactions occur along the rungs of the ladder via the oxalate bridge and weak ferromagnetic interactions along the chains. (c) 2000 Academic Press.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:437053 CAPLUS  
DN 133:171401  
TI Weaker magnetic interactions of oxalato-copper(II) binuclear compounds: synthesis, spectroscopy, crystal structure and magnetism  
AU Zhang, L.; Bu, W.-M.; Yan, S.-P.; Jiang, Z.-H.; Liao, D.-Z.; Wang, G.-L.  
CS Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China  
SO Polyhedron (2000), 19(9), 1105-1110  
CODEN: PLYHDE; ISSN: 0277-5387  
PB Elsevier Science Ltd.



DT Journal  
LA English  
AB Two binuclear copper(II) compds.,  $\text{Cu}_2(\text{tacn})_2(\mu\text{-ox})(\text{ClO}_4)_2$  (I) and  $[\text{Cu}_2(\text{bdpm})_2(\text{H}_2\text{O})_2(\mu\text{-ox})](\text{ClO}_4)_2\cdot\text{H}_2\text{O}$  (II), where tacn = 1,4,7-triazacyclononane, ox = oxalate dianion, bdpm = bis(3,5-dimethylpyrazol-1-yl)methane, were synthesized and characterized by x-ray diffraction. Each copper atom of compound I has a 4+1+1 elongated pseudo-octahedral environment; the copper atoms have a distorted square pyramidal geometry in compound II. The magnetic susceptibilities (300-4 K) indicated that the binuclear copper(II) cores were antiferromagnetically coupled ( $2J = -41 \text{ cm}^{-1}$  for compound I;  $2J = -102 \text{ cm}^{-1}$  for compound II). The weakness of the interactions for both compds. is discussed from the structural features.

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:402583 CAPLUS  
DN 133:171453  
TI Synthesis and crystal structure of oxalato-bridged dicopper(II) complex with hydrogen bonds  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{bpy})_2(\text{H}_2\text{O})_2(\text{NO}_3)_2]$   
AU Tang, J.; Gao, E.; Bu, W.; Liao, D.; Yan, S.; Jiang, Z.; Wang, G.  
CS Department of chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China  
SO Journal of Molecular Structure (2000), 525, 271-275  
CODEN: JMOSB4; ISSN: 0022-2860  
PB Elsevier Science B.V.  
DT Journal  
LA English  
AB A new dicopper(II) complex  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{bpy})_2(\text{H}_2\text{O})_2(\text{NO}_3)_2]$  (1) was synthesized and its structure determined (bpy = 2,2'-bipyridine). The structure consists of centrosym.  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{bpy})_2(\text{H}_2\text{O})_2(\text{NO}_3)_2]$  mols. with each Cu(II) ion in a distorted octahedral environment: two N atoms from bpy, two O atoms from the oxalate ion in the basal plane and two O atoms from  $\text{H}_2\text{O}$  and the nitrate group in the two axial positions. The unusual ligand arrangement in (1) and the packing of mols. are attributed to intermol. and intramol. H bonding. The intermol. and intramol. H bonding formed a H bond plane and the intermol. H bonding gave rise to a zigzag chain structure. The EPR study of the polycryst. powder at 110 K gives  $g_{\parallel} = 2.04$  and  $g_{\text{dblvert.}} = 2.20$ , typical of axially elongated Cu(II) systems, and the appearance of the half-field signals suggests a magnetic interaction between the two Cu(II) ions.

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 19 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:322811 CAPLUS  
DN 133:129163  
TI Syntheses, crystal structures and magnetic properties of chromato-, sulfato-, and oxalato-bridged dinuclear copper(II) complexes  
AU Calatayud, M. L.; Castro, I.; Sletten, J.; Lloret, F.; Julve, M.  
CS Departament de Química Inorgànica, Facultat de Química de la Universitat de Valencia, Burjassot, Valencia, 46100, Spain  
SO Inorganica Chimica Acta (2000), 300-302, 846-854  
CODEN: ICHAA3; ISSN: 0020-1693  
PB Elsevier Science S.A.  
DT Journal  
LA English  
AB Four dinuclear Cu(II) complexes  $[\text{Cu}_2(\text{bpca})_2(\text{H}_2\text{O})_3(\text{CrO}_4)]\cdot\text{H}_2\text{O}$  (1),  $[\text{Cu}_2(\text{bpca})_2(\text{H}_2\text{O})_3(\text{SO}_4)]\cdot\text{H}_2\text{O}$  (2),  $[\text{Cu}_2(\text{bpca})_2(\text{H}_2\text{O})_2(\text{C}_2\text{O}_4)]\cdot 2\text{H}_2\text{O}$  (3), and  $[\text{Cu}_2(\text{bpca})_2(\text{C}_2\text{O}_4)]$  (4) [bpca = bis(2-pyridylcarbonyl)amide anion] were synthesized and their magnetic behavior was studied as a function of temperature. The structures of 1-3 were determined by single-crystal x-ray diffraction, whereas the structure of 4 was already known. The structures of this family of complexes are made up of neutral chromate-O1,O1' (1), sulfate-O1,O1' (2) and oxalate-O1,O2:O1',O2'-bridged (3 and 4) dinuclear Cu(II) units. The two Cu atoms within the dinuclear unit of the isomorphous compds. 1 and 2 show different surroundings: they exhibit distorted square pyramidal (Cu(2)) and octahedral (Cu(1))

surroundings with the three bpca-N atoms and either a chromate (1)/sulfate (2)-O atom (Cu(2)) or a H2O-O atom (Cu(1)) defining the equatorial positions, whereas the axial sites are occupied by a H2O mol. (Cu(2) and Cu(1)) and a chromate (1)/sulfate (2)-O atom (Cu(1)). Each Cu atom of the centrosym. compound 3 is six-coordinated with the three bpca-N atoms and an oxalate-O forming the equatorial plane, whereas the axial positions are occupied by the other oxalate-O and a H2O mol. Complex 4 is also centrosym., each Cu atom exhibiting a distorted square pyramidal surrounding. The equatorial plane is the same as in 3, and an oxalate-O occupies the axial position. The intramol. Cu-Cu distances are 3.660(1) Å (1), 3.747(1) Å (2) and 5.631(1) Å (3) (5.442(1) Å in 4). The magnetic study of 1-4 reveals the occurrence of weak intramol. antiferro- (1 and 2) and ferromagnetic (3 and 4) interactions. The magnitude and nature of the magnetic coupling through these extended bridges are analyzed and discussed in light of the available structural data.

RE.CNT 57      THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5    ANSWER 20 OF 89    CAPLUS    COPYRIGHT 2006 ACS on STN  
AN    2000:292285    CAPLUS  
DN    133:98613

TI    Ascorbate oxidation leading to the formation of a catalytically active oxalato bridged dicopper(II) complex as a model for dopamine  $\beta$ -hydroxylase

AU    Thomas, Anitha M.; Mandal, Gagan C.; Tiwary, Satish K.; Rath, Rakesh K.; Chakravarty, Akhil R.

CS    Department of Inorganic & Physical Chemistry, Indian Institute of Science, Bangalore, 560012, India

SO    Dalton (2000), (9), 1395-1396  
CODEN: DALTFG

PB    Royal Society of Chemistry

DT    Journal

LA    English

AB    The dicopper(II) complexes  $[\text{Cu}_2(\text{bpy})_2(\mu\text{-ox})]\text{X}_2$  ( $\text{X} = \text{ClO}_4^-$ ,  $\text{PF}_6^-$ ;  $\text{ox} = \text{C}_2\text{O}_4^{2-}$ ) were prepared and the  $\text{PF}_6^-$  salt was characterized by x-ray crystallog. (monoclinic, space group  $\text{C}_2/\text{m}$ ,  $\text{R}_1 = 0.0357$ ). The complexes are catalytically active in the oxidation of ascorbic acid by dioxygen involving a copper(I) intermediate species and the process is also effective in the presence of benzylamine to form benzaldehyde.

RE.CNT 15      THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5    ANSWER 21 OF 89    CAPLUS    COPYRIGHT 2006 ACS on STN  
AN    2000:177820    CAPLUS  
DN    132:287929

TI    Synthesis and magnetic properties of one-dimensional metal oxalate networks as molecular-based magnets

AU    Singh, B. P.; Singh, B.

CS    Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi, 221 005, India

SO    Bulletin of Materials Science (2000), 23(1), 11-16  
CODEN: BUMSDW; ISSN: 0250-4707

PB    Indian Academy of Sciences

DT    Journal

LA    English

AB    The homo- and heteropolymetallic assemblies of  $\text{MM}'(\text{OX})_2(\text{H}_2\text{O})_4$ , where  $\text{MM}'$  represents  $\text{MnMn}$ ,  $\text{CoMn}$ ,  $\text{NiMn}$ ,  $\text{CuMn}$ ,  $\text{CoCo}$ ,  $\text{NiCo}$ ,  $\text{CuCo}$ ,  $\text{NiNi}$ ,  $\text{CuNi}$ , and  $\text{CuCu}$ , and  $\text{OX} = \text{oxalato}$  (1-10), were prepared by reacting metal(II) salts of Mn, Co, Ni, and Cu and K oxalate monohydrate in hot  $\text{H}_2\text{O}$  (90-100°). The magnetic susceptibility data of 8 and 9 in the 300 K-20 K temperature range obeys the Curie-Weiss law and exhibits Weiss consts. -50 K and -100 K, resp. On lowering the temperature, the effective magnetic moment decreases gradually and is indicative of antiferromagnetic phase transition. The complexes also were characterized by ES mass spectrometry, IR, electronic, and ESR spectra.

RE.CNT 16      THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:749937 CAPLUS  
DN 132:101948  
TI Synthesis, spectral and magnetic characterisation of copper(II) dinuclear  
and polynuclear complexes with a macrocyclic 34-membered hexaamine  
AU Pietraszkiewicz, Marek; Pietraszkiewicz, Oksana; Saf, Robert; Hummel,  
Klaus; Skorupa, Anna; Mrozinski, Jerzy  
CS Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw,  
01-224, Pol.  
SO Journal of Inclusion Phenomena and Macrocyclic Chemistry (1999),  
35(1-2), 233-242  
CODEN: JIPCF5  
PB Kluwer Academic Publishers  
DT Journal  
LA English  
AB 34-Membered macrocyclic hexaamine containing two independent N3 donor sets  
forms homodinuclear copper(II) complexes. Displacements of anions within  
the copper(II) chloride complexes occurred easily upon addition of different  
anions to the CuCl2 complex. All new complexes were characterized by  
elemental anal., IR, UV/visible spectroscopy, and magnetic susceptibility  
measurements. Tetranuclear complexes indicate relation  $\chi_{Cu-1}$  vs. T in  
agreement with the Curie-Weiss law. A behavior anomalous in relation to  
the phthalate complexes is shown by the [Cu4L2Cl4(ox)2] complex in which  
an antiferromagnetic coupling ( $J = -53.9$  cm<sup>-1</sup>) between the Cu<sup>2+</sup> ions  
through the C2O4<sup>2-</sup> bridge is observed  
RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 23 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:673859 CAPLUS  
DN 132:8461  
TI Synthesis and characterization of binuclear  $\mu$ -oxalato nickel(II),  
copper(II) and zinc(II) complexes with 3,3'-diamino-N-methyl-dipropylamine  
or trans-1,2-diaminocyclohexane  
AU Smekal, Zdenek; Travnicek, Zdenek; Lloret, Francesc; Marek, Jaromir  
CS Department of Inorganic and Physical Chemistry, Palacky University,  
Olomouc, 771 47, Czech Rep.  
SO Polyhedron (1999), 18(21), 2787-2793  
CODEN: PLYHDE; ISSN: 0277-5387  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB New binuclear complexes [(Ni(Medpt)NO3)2ox] (1) (Medpt =  
3,3'-diamino-N-methyl-dipropylamine, H2ox = oxalic acid),  
[(Ni(dach)2)2ox]NO3·2H2O (2) (dach = trans-1,2-diaminocyclohexane),  
[(Cu(Medpt))2ox]X2·yH2O (X = NO3, y = 2 2/3 (3); X=ClO4, y = 0 (4))  
and [(Zn(dach)2)2ox](ClO4)2·2H2O (5) were prepared and characterized  
by IR and UV-visible spectroscopies. Spectroscopic data are consistent  
with oxalate-bridged structures between six-coordinated (N3O3 or N4O2)  
Ni(II) (compds. 1 or 2), five-coordinated (N3O2) Cu(II) (compds. 3 and 4)  
or six-coordinated (N4O2) Zn(II) (compound 5). The crystal structure of 3  
was determined by single-crystal x-ray anal. The structure of 3 consists of  
centrosym. binuclear cations [(Medpt)Cu(ox)Cu(Medpt)]<sup>2+</sup>, nitrate anions  
and H2O mols. of crystallization. The Cu atom is five-coordinated by two oxalate-O  
and three Medpt-N atoms, in a hybrid arrangement between  
trigonal-bipyramidal and square-pyramidal. The temperature dependence of  
magnetic susceptibility (1.8-300 K) was measured for compds. 1-4.  
Magnetochem. measurements show that Ni(II) complexes are  
antiferromagnetically coupled,  $J = -29.4$  (1) and  $-32.7$  cm<sup>-1</sup> (2) ( $H =$   
 $-JS_1S_2$ ) while the Cu(II) complexes present a very weak coupling,  $J = -2.6$   
(3) and  $+1.9$  cm<sup>-1</sup> (4), being antiferro- and ferromagnetic, resp.  
RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 24 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:314534 CAPLUS  
DN 131:38799  
TI Synthesis, chemical characterization, X-ray crystal structure and magnetic  
properties of oxalato-bridged copper(II) binuclear complexes with

2,2'-bipyridine and diethylenetriamine as peripheral ligands  
AU Castillo, Oscar; Muga, Inaki; Luque, Antonio; Gutierrez-Zorrilla, Juan M.;  
Sertucha, Jon; Vitoria, Pablo; Roman, Pascual  
CS Departamento de Quimica Inorganica, Universidad del Pais Vasco, Bilbao,  
E-48080, Spain  
SO Polyhedron (1999), 18(8,9), 1235-1245  
CODEN: PLYHDE; ISSN: 0277-5387  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB Two new  $\mu$ -oxalato binuclear Cu(II) complexes,  
[ $\{Cu(NO_3)(H_2O)(bipy)\}_2(ox)$ ] (1) and [ $\{Cu(dien)\}_2(ox)(NO_3)_2$ ] (2), with ox =  
oxalate, dien = diethylenetriamine and bipy = 2,2'-bipyridine, were  
synthesized and their crystal and mol. structures were determined by  
single-crystal x-ray diffraction methods. The crystal structure of 1  
consists of centrosym. neutral dimers where the Cu atoms lie in a strongly  
elongated octahedral environment, surrounded by two N atoms of a bipy mol.  
and two O atoms of the bridging oxalato group in the equatorial plane and  
O atoms of H<sub>2</sub>O mols. and nitrate ions in the axial positions. Crystal  
structure of 2 is made up of noncoordinated nitrate anions and asym.  
binuclear cations in which Cu atoms are in a distorted square-pyramidal  
coordination with three atoms of a diethylenetriamine ligand and an O atom  
of the asym. coordinated oxalato bridge building the basal plane and the  
other O atom of the oxalato ligand filling the apical position. Both  
compds. were also characterized by FTIR and ESR spectroscopies, thermal  
anal. and variable temperature magnetic susceptibility measurements. The two  
compds. exhibit antiferromagnetic exchange with a singlet-triplet separation of  
-382 and -6.5 cm<sup>-1</sup> for 1 and 2, resp. Magnetic and ESR results are  
discussed with respect to the crystal structure of the compds.  
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 25 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:297682 CAPLUS  
DN 131:96274  
TI Theoretical study of the exchange coupling in copper(II) binuclear  
compounds with oxamate and related polyatomic bridging ligands  
AU Cano, Joan; Ruiz, Eliseo; Alemany, Pere; Lloret, Francesc; Alvarez,  
Santiago  
CS Departament de Quimica Inorganica, Universitat de Valencia, Burjassot,  
Spain  
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry  
(1999), (10), 1669-1676  
CODEN: JCOTBI; ISSN: 0300-9246  
PB Royal Society of Chemistry  
DT Journal  
LA English  
AB A theor. d. functional study of the exchange coupling was carried out for  
binuclear Cu(II) compds. with oxamate and related bridging ligands:  
oxalate, oxamate, ethylenetetraamdate, dithiooxamate, dithiooxalate,  
tetrathiooxalate, bipyrimidine, and bisimidazole. Model calcns. were used  
to examine the influence of the donor atoms at the bridging ligand and of  
the ligands' orientation on the coupling constant. Ests. for the  
singlet-triplet gap of complete structures of cis- and  
trans-oxamato-bridged complexes are reported. Comparison of these  
results with those obtained from qual. models provides some insight into  
the limits of applicability of these methods for the study of  
magneto-structural correlations.  
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 26 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:126186 CAPLUS  
DN 130:245634  
TI Synthesis, Crystal Structure, and Magnetic Properties of  
Oxalato-Copper(II) Complexes with 3,3-Bis(2-imidazolyl)propionic Acid, an  
Imidazole-Carboxylate Polyfunctional Ligand: From Mononuclear Entities to  
Ladder-Like Chains  
AU Akhriff, Y.; Server-Carrio, J.; Sancho, A.; Garcia-Lozano, J.; Escriva,

E.; Folgado, J. V.; Soto, L.  
CS Departament de Química Inorgànica, Universitat de Valencia, Burjassot,  
46100, Spain  
SO Inorganic Chemistry (1999), 38(6), 1174-1185  
CODEN: INOCAJ; ISSN: 0020-1669  
PB American Chemical Society  
DT Journal  
LA English  
AB The synthesis of five new Cu(II) compds. [Cu(HBIP)(C2O4)]·H2O (1),  
[Cu(HBIP)(C2O4)(OH2)]·2H2O (2), [{Cu(HBIP)Cl}2(μ-C2O4)]·2H2O (3), [{Cu(BIP)}2(μ-C2O4)]·2H2O (4) and  
[{Cu(BIP)}2(μ-C2O4)]·6H2O (5), together with their spectral and  
magnetic characterization, is reported. Crystal structures of compds. 2,  
3 and 5 were solved. All these compds. crystallize in the triclinic  
system, space group P.hivin.1, with a 7.3322(3), b 10.014(1), c 11.541(1)  
Å, α 113.22(1), β 91.37(1), γ 94.51(1)°, Z = 2  
for compound 2; a 7.444(2), b 8.518(2), c 11.231(2) Å, α 97.45(2),  
β 98.99(2), γ 97.95(2)°, Z = 1 for compound 3; and a  
7.977(1), b 8.656(1), c 11.807(1) Å, α 69.06(1), β  
86.07(1), γ 67.36(1)°, Z = 1 for compound 5. In compound 2 the  
asym. unit consists of one isolated neutral [Cu(HBIP)(C2O4)(OH2)] mol. and  
two noncoordinated H2O mols. The Cu(II) ion is five-coordinated (4+1  
coordination mode) with HBIP and oxalato entities acting as bidentate  
ligands and the axial H2O mol. as the 5th ligand. The structure of compound  
3 is made up of centrosym. binuclear [{Cu(HBIP)(Cl)}2(μ-C2O4)] units  
and noncoordinated H2O mols. The two Cu atoms are linked through a  
bis-bidentate oxalato group leading to a metal-metal separation of 5.28(3)  
Å. The coordination stereochem. of the CuN2O2Cl chromophore is  
approx. SP. Compound 5 exhibits a structure built of ladder-like chains.  
In these chains the rungs are constituted by the neutral dinuclear  
centrosym. [(BIP)Cu(C2O4)Cu(BIP)] entities. The oxalato group bridges two  
Cu atoms in a bis-bidentate fashion, whereas the BIP acts as a tridentate  
ligand, connecting through their carboxylate groups these dimeric units  
along the a axis. The Cu atom is involved in a five-coordinated CuN2O2O'  
chromophore, with a coordination geometry intermediate between SP and TBP.  
The magnetic properties of all complexes were studied. Compound 1 and 2  
follow a Curie-Weiss law with very low values of θ. The other three  
compds. exhibit an antiferromagnetic coupling, with 2J = -265 cm-1 for 3,  
2J = -108 cm-1 for 4, and 2J = -5.7 cm-1 for 5. The strength of the  
exchange interaction is discussed from the structural features and  
correlated with published magneto-structural data on similar  
oxalato-bridged Cu(II) compds.

RE.CNT 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 27 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:124784 CAPLUS  
DN 130:189668  
TI Crystal structure of the binuclear copper(II) complex [Cu2(tacn)2(μ-ox)](ClO4)2 (tacn = 1,4,7-triazacyclononane)  
AU Zhang, L.; Yan, H.-L.; Yan, S.-P.; Jiang, Z.-H.; Liao, D.-Z.; Wang, G.-L.  
CS Department of Chemistry, Nankai University, Tianjin, 300071, Peop. Rep. China  
SO Polish Journal of Chemistry (1999), 73(2), 391-394  
CODEN: PJCHDQ; ISSN: 0137-5083  
PB Polish Chemical Society  
DT Journal  
LA English  
AB The title compound is triclinic, space group P.hivin.1, with a 10.0302(6), b 10.8335(6), c 11.5471(9) Å, α 96.693(5), β 97.441(6), and γ 97.714(5)°; dc = 1.828, Z = 2, R = 0.0443, rw = 0.0509 for 4041 reflections. The geometries around the 2 Cu ions are identical inside exptl. error, and considered that each Cu ion has a distorted square pyramidal environment with 2 N atoms of tacn and 2 O atoms of oxalato bridge in the basal plane CuN2O2, and the 3rd N atom of tacn occupying the apical position. Bond lengths and bond angles are given and discussed.

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 28 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1998:771517 CAPLUS  
 DN 130:118608  
 TI Structure and magnetic properties of an oxalic acid-bridged dinuclear copper(II) complex  
 AU Saha, Manas Kumar; Sen, Sutapa; Kundu, Parimal; Gupta, Tarakranjan; Gramlich, Volker; Mitra, Samiran  
 CS Department Chemistry, Jadavpur University, Calcutta, 700032, India  
 SO Zeitschrift fuer Naturforschung, B: Chemical Sciences (1998), 53(11), 1281-1284  
 CODEN: ZNBSEN; ISSN: 0932-0776  
 PB Verlag der Zeitschrift fuer Naturforschung  
 DT Journal  
 LA English  
 AB [LCu{ $\mu$ -(OH)<sub>2</sub>(C<sub>2</sub>O<sub>2</sub>)}CuL](ClO<sub>4</sub>)<sub>2</sub> (HL = 3-(dimethylaminopropyl)salicylaldehyde) was synthesized and its crystal structure was determined C<sub>26</sub>H<sub>36</sub>Cl<sub>2</sub>Cu<sub>2</sub>N<sub>4</sub>O<sub>14</sub>, triclinic space group P<sub>2</sub><sub>1</sub>h<sub>1</sub> with a = 9.288(9), b = 10.016(11), c = 10.09(2) Å, α = 101.05(11), β = 108.22(10), γ = 110.22(10)°, V = 787(2) Å<sup>3</sup>, Z = 2, ρ<sub>c</sub> = 1.744 g/cm<sup>3</sup>, μ(MoKα) = 1.597 mm<sup>-1</sup>, F(000) = 424, 1168 independent reflections, 223 refined parameters, R<sub>1</sub> = 0.0282, wR<sub>2</sub> = 0.0637 (I > 2σ(I)). Two Cu<sup>2+</sup> ions in a distorted square-planar coordination are bridged by an oxalate to form dinuclear units. The Cu<sup>2+</sup> centers are separated by 5.2 Å and antiferromagnetically coupled (J = -478 cm<sup>-1</sup>), which follows from temperature-dependent magnetic susceptibility measurements at 12-300 K.

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 29 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1998:735167 CAPLUS  
 DN 130:42583  
 TI Mildew cleaning compositions with good storability, lasting effects, and no irritating odor  
 IN Nishino, Takashi; Kishi, Minoru; Yamamoto, Nobuyuki; Kubozono, Takayasu  
 PA Lion Corp., Japan  
 SO Jpn. Kokai Tokkyo Koho, 13 pp.  
 CODEN: JKXXAF

DT Patent  
 LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 10298592	A2	19981110	JP 1997-320470	19971106 <--
PRAI	JP 1997-62272	A	19970228		

OS MARPAT 130:42583

AB The title compns. contain peroxy compds. and metal complexes having organic macrocyclic ligands. An aqueous composition comprised H<sub>2</sub>O<sub>2</sub> 5, N,N,N',N'-tetraacetylenediamine 1, tris-μ-oxobis(1,4,7-trimethyl-1,4,7-triazacyclononane)manganese(IV) hexafluorophosphate 0.01, and K<sub>2</sub>CO<sub>3</sub> 5%.

L5 ANSWER 30 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1998:542391 CAPLUS  
 DN 129:224904  
 TI Synthesis and characterization of (μ-oxalato)nickel(II), copper(II) and zinc(II) complexes with chelating polyamines  
 AU Smekal, Zdenek; Travnicek, Zdenek; Nadvornik, Milan; Sindelar, Zdenek; Klicka, Roman; Marek, Jaromir  
 CS Department of Inorganic and Physical Chemistry, Palacky University, Olomouc, 771 47, Czech Rep.  
 SO Collection of Czechoslovak Chemical Communications (1998), 63(6), 783-792  
 CODEN: CCCCAK; ISSN: 0010-0765  
 PB Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic  
 DT Journal  
 LA English  
 AB New binuclear complexes [(Ni(aep)<sub>2</sub>)<sub>2</sub>ox](ClO<sub>4</sub>)<sub>2</sub> (1) (aep =

2-(2-aminoethyl)pyridine, H<sub>2</sub>ox = oxalic acid), [(Ni(ept)H<sub>2</sub>O)<sub>2</sub>ox](NO<sub>3</sub>)<sub>2</sub> (2), (ept = N-(2-aminoethyl)-1,3-diaminopropane), [(Cu(aep)H<sub>2</sub>O)<sub>2</sub>ox](ClO<sub>4</sub>)<sub>2</sub> (3), [(Cu(ept))<sub>2</sub>ox](NO<sub>3</sub>)<sub>2</sub>.H<sub>2</sub>O (4) and [(Zn(L))<sub>2</sub>ox](ClO<sub>4</sub>)<sub>2</sub>.nH<sub>2</sub>O (L = ept, n = 0 (5); L = N,N'-bis(3-aminopropyl)-1,2-diaminoethane (3,2,3-tet), n = 4 (6)) were prepared and studied by IR and UV-visible spectroscopies. Spectroscopic data are consistent with oxalato-bridged structures between six-coordinate (N<sub>4</sub>O<sub>2</sub> or N<sub>3</sub>O<sub>3</sub>) Ni(II) (compds. 1 and 2), (N<sub>2</sub>O<sub>3</sub> or N<sub>3</sub>O<sub>2</sub>) Cu(II) (compds. 3 and 4) or (N<sub>3</sub>O<sub>2</sub> or N<sub>4</sub>O<sub>2</sub>) Zn(II) (compds. 5 and 6). The crystal structure of 3 was determined by single-crystal x-ray anal. The Cu atom is coordinated by two O atoms of the oxalato ligand, two N atoms belonging to aep and one O atom of H<sub>2</sub>O in a square-pyramidal arrangement. The intermetallic distance of Cu(I)-Cu(1a) is 5.204(2) Å. The temperature dependence of magnetic susceptibilities (94-298 K) was measured for 1 and 3. Magnetochem. measurements show that metal ions in these compds. are antiferromagnetically coupled, J = -17 and -160 cm<sup>-1</sup> (H = -2JS<sub>1</sub>S<sub>2</sub>) for 1 and 3, resp.

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 31 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1998:172020 CAPLUS

DN 128:238475

TI Copper(II) diethylenetriamine perchlorate complexes bridged through varying length dicarboxylato spacers: synthesis, characterization and EPR studies

AU Subramanian, P. S.; Dave, Paresh C.; Boricha, Vinod P.; Srinivas, D.

CS Sophisticated Analytical Instruments Laboratory, Central Salt and Marine Chemicals Research Institute, Bhavnagar, 364 002, India

SO Polyhedron (1998), 17(4), 443-448

CODEN: PLYHDE; ISSN: 0277-5387

PB Elsevier Science Ltd.

DT Journal

LA English

AB The synthesis and spectral characterization of dinuclear copper(II) complexes [(dien)Cu<sub>2</sub>(dien)](ClO<sub>4</sub>)<sub>2</sub>, where dien = diethylenetriamine and L<sub>2</sub>- = oxalato, malonato, succinato, phthalato, isophthalato and terephthalato, are reported. IR spectra reveal that the mode of carboxylato coordination is anti-anti for oxalato complexes while it adopts chelate or polymeric syn-anti coordination for the rest of the complexes. The stereochem. around copper is distorted square pyramidal. Oxalato forms two types of complexes I and II. EPR for I was characterized by a rhombic g tensor with g<sub>3</sub> < g<sub>1</sub> and g<sub>2</sub> and suggest that the unpaired electron has a predominant dz<sup>2</sup> character while II and the rest of the dicarboxylato complexes were characterized by an axial g tensor (g<sub>1</sub> > g<sub>2</sub> > g<sub>3</sub>) suggesting the occupancy of unpaired electron in a dx<sup>2</sup>-y<sup>2</sup> orbital. Frozen solution EPR spectra at 77 K indicate that the solvent mol. coordinates with the metal ion. Magnetic exchange in these complexes is intramol. and both conjugated and unconjugated spacer dicarboxylato ligands propagate the exchange between the metal ions.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 32 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:793812 CAPLUS

DN 128:96682

TI Magnetic susceptibility of [Cu<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub> - a candidate for a spin ladder compound

AU Honda, Zentaro; Nonomura, Yoshihiko; Katsumata, Koichi

CS The Institute of Physical and Chemical Research (RIKEN), Saitama, 351-01, Japan

SO Journal of the Physical Society of Japan (1997), 66(11), 3689-3690

CODEN: JUPSAU; ISSN: 0031-9015

PB Physical Society of Japan

DT Journal

LA English

AB Magnetic susceptibility of [Cu<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub> was measured as a function of temperature A broad peak is observed around 300 K and a Curie tail is

observed at lower temps. The diamagnetic susceptibility was determined A spin gap is observed This material acts like a 2-leg spin ladder compound  
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 33 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1997:198075 CAPLUS  
DN 126:206773  
TI Reduction and Aerobic Oxidation of Hexaketocyclohexane (C6O6) by Reaction with Metallic Copper  
AU Speier, Gabor; Speier, Edit; Noll, Bruce; Pierpont, Cortlandt G.  
CS Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309, USA  
SO Inorganic Chemistry (1997), 36(7), 1520-1521  
CODEN: INOCAJ; ISSN: 0020-1669  
PB American Chemical Society  
DT Journal  
LA English  
AB Cyclic C6O6 was reacted with metallic copper as a potential route to rhodizonate complexes of Cu(II). The product isolated under aerobic conditions was found from crystallog. anal. to contain croconate C5O52- and oxalate C2O42- ligands bridging CuII(tmeda) centers in a linear polymer [(tmeda)Cu(μ-C5O5)Cu(tmeda)(μ-C2O4)]<sub>n</sub> (crystal data: monoclinic, space group C2/c, a 17.036(3), b 12.630(3), c 12.897(3) Å, β 117.41(3)°, Z = 4, R = 0.049, and R<sub>w</sub>(F<sub>2</sub>) = 0.092). Oxalate ligands are believed to result from O<sub>2</sub> addition to a CuI(C6O6•-) species, formed initially in the reaction, in steps that give C5O52- and CO2•- radical anion by elimination and ring contraction.

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 34 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1997:122647 CAPLUS  
DN 126:206757  
TI Synthesis, structure and magnetic properties of oxalate-bridged complex [Cu<sub>2</sub>(bpy)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>][Cu(bpy)(C<sub>2</sub>O<sub>4</sub>)](NO<sub>3</sub>)<sub>2</sub>  
AU Shi, Juan; Yang, Guang-Ming; Cheng, Peng; Liao, Dai-Zheng; Jiang, Zong-Hui; Wang, Geng-Lin  
CS Dep. Chem., Nankai Univ., Tianjin, Peop. Rep. China  
SO Polyhedron (1996), Volume Date 1997, 16(3), 531-534  
CODEN: PLYHDE; ISSN: 0277-5387  
PB Elsevier  
DT Journal  
LA English  
AB [Cu<sub>2</sub>(bpy)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>][Cu(bpy)(C<sub>2</sub>O<sub>4</sub>)](NO<sub>3</sub>)<sub>2</sub> was synthesized by electrophilic attack of [Cu(bpy)(H<sub>2</sub>O)<sub>2</sub>]<sup>2+</sup> on K<sub>3</sub>[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>] (bpy stands for 2,2'-bipyridyl). The crystal structure of the complex consists of binuclear [Cu<sub>2</sub>(bpy)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>]<sup>2+</sup> and mononuclear [Cu(bpy)(H<sub>2</sub>O)(C<sub>2</sub>O<sub>4</sub>)]. The temperature dependences of the magnetic susceptibilities of the complex were studied in the 4.2-300 K range, giving the exchange integral J = -340 cm<sup>-1</sup>, indicating rather strong antiferromagnetic interaction between the Cu(II) ions within the binuclear unit.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 35 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1997:120586 CAPLUS  
DN 126:180397  
TI Structurally alternating copper(II) chains from oxalate and azide bridging ligands: syntheses and crystal structure of [Cu<sub>2</sub>(μ-ox)(deen)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(ClO<sub>4</sub>)<sub>2</sub>] and [{Cu<sub>2</sub>(μ-N<sub>3</sub>)(μ-ox)(deen)<sub>2</sub>}]<sub>n</sub>[ClO<sub>4</sub>]<sub>n</sub> (deen = Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>)  
AU Vicente, Ramon; Escuer, Albert; Ferretjans, Joan; Stoeckli-Evans, Helen; Solans, Xavier; Font-Bardia, Merce  
CS Departament de Química Inorgànica, Universitat de Barcelona, Barcelona, 08028, Spain  
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1997), (2), 167-171  
CODEN: JCDTBI; ISSN: 0300-9246



PB Royal Society of Chemistry  
DT Journal  
LA English  
AB The  $\mu$ -oxalato dinuclear compound  $[\text{Cu}_2(\mu\text{-ox})(\text{deen})_2(\text{H}_2\text{O})_2(\text{ClO}_4)_2]$  1 and the derived alternating  $\mu$ -oxalato- $\mu$ -azido chain  $[\{\text{Cu}_2(\mu\text{-N}_3)(\mu\text{-ox})(\text{deen})_2\}_n][\text{ClO}_4]_n$  2, where deen = N,N-diethylethane-1,2-diamine, were synthesized and characterized. The crystal structures of 1 and 2 were determined by single-crystal x-ray anal. Their magnetic behavior was recorded between 300 and 4 K, showing strong antiferromagnetic coupling in each case. The data were fitted by the expression for a dinuclear Cu(II) compound giving the parameters  $J = -300(3) \text{ cm}^{-1}$ ,  $g = 2.15(1)$  for 1 and  $J = -287(1) \text{ cm}^{-1}$ ,  $g = 2.28(1)$  for 2.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 36 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1996:678794 CAPLUS  
DN 126:13985  
TI Copper(II) Complexes of the Hexaaza Macrocyclic Ligand  
3,6,9,16,19,22-Hexaaza-27,28-dioxatricyclo [ 22.2.1.111,14 ] octacosa-1  
(26) ,11 ,13 ,24 - tetraene and Their Interaction with Oxalate, Malonate,  
and Pyrophosphate Anions. [Erratum to document cited in CA124:276917]  
AU Lu, Qin; Reibenspies, Joseph H.; Martell, Arthur E.; Motekaitis, Ramunas  
J.  
CS Department of Chemistry, Texas A and M University, College Station, TX,  
77843-3255, USA  
SO Inorganic Chemistry (1996), 35(25), 7462  
CODEN: INOCAJ; ISSN: 0020-1669  
PB American Chemical Society  
DT Journal  
LA English  
AB The authors refined the structure of CAS Registry number 175613-61-3  
. The have published supporting information. The errors were not  
reflected in the abstract or the index entries.

L5 ANSWER 37 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1996:279237 CAPLUS  
DN 125:24803  
TI Synthesis, magnetic behavior and structural characterization of the  
alternating hexanuclear copper(II) compound  $[\text{Cu}_6(\text{tmen})_6(\mu\text{-N}_3)_2(\mu\text{-C}_2\text{O}_4)_3(\text{H}_2\text{O})_2][\text{ClO}_4]_4 \cdot 2\text{H}_2\text{O}$  (tmen =  $\text{Me}_2\text{NCH}_2\text{CH}_2\text{NMe}_2$ )  
AU Vicente, Ramon; Escuer, Albert; Solans, Xavier; Font-Bardia, Merce  
CS Dep. Quimica Inorganica, Univ. Barcelona, Barcelona, 08028, Spain  
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry  
(1996), (9), 1835-1838  
CODEN: JC DTBI; ISSN: 0300-9246  
PB Royal Society of Chemistry  
DT Journal  
LA English  
AB  $[\text{Cu}_6(\text{tmen})_6(\mu\text{-N}_3)_2(\mu\text{-C}_2\text{O}_4)_3(\text{H}_2\text{O})_2][\text{ClO}_4]_4 \cdot 2\text{H}_2\text{O}$  (1; tmen =  
N,N,N',N'-tetramethyl-ethane-1,2-diamine) was synthesized and  
characterized. Its crystal structure was determined by single-crystal x-ray  
anal. The magnetic behavior was recorded between 300 and 4 K, showing  
strong antiferromagnetic coupling. The magnetic susceptibility data were  
fitted by the expression for a dinuclear Cu(II) compound giving the  
parameters  $J = -289(2) \text{ cm}^{-1}$ ,  $g = 2.03(1)$ . Polycryst. powder ESR spectra  
were recorded at variable temperature The broad room-temperature signal having  $g =$   
2.12 vanished at .apprx.55 K.

L5 ANSWER 38 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1996:202976 CAPLUS  
DN 124:276917  
TI Copper(II) Complexes of the Hexaaza Macrocyclic Ligand  
3,6,9,16,19,22-Hexaaza-27,28-dioxatricyclo[22.2.1.111,14]octacosa-1(26),  
11,13,24-tetraene and Their Interaction with Oxalate, Malonate, and  
Pyrophosphate Anions  
AU Lu, Qin; Reibenspies, Joseph J.; Martell, Arthur E.; Motekaitis, Ramunas  
J.  
CS Department of Chemistry, Texas A and M University, College Station, TX,

77843-3255, USA

SO Inorganic Chemistry (1996), 35(9), 2630-6  
CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

AB The hexaaza macrocyclic ligand 3,6,9,16,19,22-hexaaza-27,28-dioxatricyclo[22.2.1.111,14]octacos-1(26),11,13,24-tetraene (BFBD), forms both mono- and dinuclear complexes, as well as several protonated and hydroxo chelates, with Cu(II) ions. These cationic species can bind inorg. and organic anions through coordination and H bonding. Stability consts. of the mono- and dinuclear Cu(II) complexes of BFBD and their interaction with oxalate, malonate, and pyrophosphate anions were measured potentiometrically. The nature of the bonding between the hosts and the guests is discussed. The crystal structures of two new dinuclear Cu(II) complexes, determined by x-ray crystallog., are also reported. [BFBD<sub>2</sub>Cu<sub>2</sub>(Cl)<sub>3</sub>](ClO<sub>4</sub>·0.5H<sub>2</sub>O) crystallizes in the monoclinic system, space group P2<sub>1</sub>/n, with a 13.267(2), b 12.155(6), c 18.461 0 Å, β 90.86(2)°, and Z = 4. Each Cu(II) ion is coordinated by three N atoms from the diethylenetriamine unit of the macrocyclic ligand and two chloride anions, forming a square pyramidal geometry. [BFBD<sub>2</sub>Cu<sub>2</sub>(Ox)](BF<sub>4</sub>)·1.8ClO<sub>4</sub>·2 crystallizes in the triclinic system, space group P1, with a 6.772(1), b 10.646(2), c 11.517(2) Å, α 64.74(3), β 79.79(3), γ 81.94(3)°, and Z = 1. The environment of each Cu is intermediate between square pyramidal and trigonal pyramidal. The oxalate anion bridges in a bis-bidentate fashion between two Cu(II) ions.

L5 ANSWER 39 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:931687 CAPLUS

DN 124:20341

TI Magnetic Exchange through Oxalate Bridges: Synthesis and Characterization of (μ-Oxalato)dimetal(II) Complexes of Manganese, Iron, Cobalt, Nickel, Copper, and Zinc

AU Glerup, Jorgen; Goodson, Patricia A.; Hodgson, Derek J.; Michelsen, Kirsten

CS Chemistry Laboratory I, H. C. Oersted Institute, Copenhagen, DK-2100, Den.

SO Inorganic Chemistry (1995), 34(25), 6255-64  
CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

AB The syntheses and characterization of binuclear μ-oxalato complexes [(N)<sub>4</sub>M(C<sub>2</sub>O<sub>4</sub>)M(N)<sub>4</sub>]<sup>2+</sup>, where M is MnII, FeII, CoII, NiII, CuII, and ZnII, are described. The ligands (N)<sub>4</sub> represent the tetradentate ligands N,N'-bis(2-pyridylmethyl)-1,2-ethanediamine (bispicen, C<sub>14</sub>H<sub>18</sub>N<sub>4</sub>), N,N'-bis(2-pyridylmethyl)-1,3-propanediamine (bispicn, C<sub>15</sub>H<sub>20</sub>N<sub>4</sub>), and N,N'-bis(2-pyridylmethyl)-N,N'-dimethyl-1,2-ethanediamine (bispicMe<sub>2</sub>en, C<sub>16</sub>H<sub>22</sub>N<sub>4</sub>). The crystal structures of five representative complexes were determined. The Mn complex [(bispicen)Mn(C<sub>2</sub>O<sub>4</sub>)Mn(bispicen)](ClO<sub>4</sub>)<sub>2</sub> (1a) crystallizes in the noncentrosym. orthorhombic space group Pna2<sub>1</sub> with four binuclear formula units with a = 21.771(4), b = 23.650(5), and c 7.328(2) Å. The corresponding Fe(II), Cu(II), and Zn(II) complexes (2a, 5a, and 6a, resp.) are isomorphous with this Mn complex 1a. [(BispicMe<sub>2</sub>en)Mn(C<sub>2</sub>O<sub>4</sub>)Mn(bispicMe<sub>2</sub>en)](ClO<sub>4</sub>)<sub>2</sub> (1c) crystallizes in the centrosym. monoclinic space group P2<sub>1</sub>/c with two binuclear formula units with a 9.218(2) Å, b 13.189(2) Å, c 17.213(3) Å, and β 92.780(10)°. The Co complex [(bispicen)Co(C<sub>2</sub>O<sub>4</sub>)Co(bispicen)](ClO<sub>4</sub>)<sub>2</sub>·H<sub>2</sub>O (3a) crystallizes in the triclinic space group P.hivin.1 with one binuclear formula unit with a 8.832(2) Å, b 9.297(2) Å, c 13.045(3) Å, α 108.01(3), β 98.48(3), and γ 93.31(3)°. The corresponding Ni(II) analog, 4a, is isomorphous with this Co complex. The Cu(II) complex [(bispicen)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(bispicen)](ClO<sub>4</sub>)<sub>2</sub> (5a) is isomorphous with 1a: a 21.531(4), b 23.708(5), and c 7.186(1) Å. The Cu(II) complex [(bispicMe<sub>2</sub>en)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(bispicMe<sub>2</sub>en)](ClO<sub>4</sub>)<sub>2</sub> (5c) crystallizes in the centrosym. monoclinic space group P2<sub>1</sub>/n with two binuclear formula units with a 8.089(2) Å, b 22.001(4) Å, c 12.179(2) Å, and β 107.93(3)°. The corresponding Co(II), Ni(II), and Zn(II) complexes (3c, 4c, and 6c, resp.) are

isomorphous with this Cu complex. All five complexes contain six-coordinate metal centers bridged by planar bis-bidentate oxalate groups. The J-values for these oxalato bridged metal complexes are .apprx.2, 6, 10, 33, and 2 cm<sup>-1</sup> for MnII, FeII, CoII, NiII, and CuII, resp. This is explained as a result of the magnetic interaction between the x<sup>2</sup>-y<sup>2</sup> orbitals on the two metal atoms, and in spite of the difference between the J-values for these complexes the interaction matrix element between these orbitals have approx. the same value for the MnII, FeII, CoII, and NiII complexes. The small J-values for the CuII complexes are caused by the fact that in these cases the x<sup>2</sup>-y<sup>2</sup> orbitals are not the magnetic orbitals.

L5 ANSWER 40 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:842825 CAPLUS  
 DN 123:274300  
 TI Synthesis, Crystal Structure, Optical and Magnetic Properties of a Novel Two-Dimensional Copper(II) Network formed conjointly with  $\mu$ -Bipyrimidine,  $\mu$ -Oxalato, and  $\mu$ -Chloro Ligands  
 AU Decurtins, Silvio; Schmalle, Helmut W.; Schneuwly, Philippe; Zheng, Li-Min; Ensling, Juergen; Hauser, Andreas  
 CS Institut fuer Anorganische Chemie, Universitaet Zuerich, Zurich, CH-8057, Switz.  
 SO Inorganic Chemistry (1995), 34(22), 5501-6  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB The preparation, x-ray crystal structure, and optical and magnetic properties of a polymeric two-dimensional  $\mu$ -2,2'-bipyrimidine (C<sub>8</sub>H<sub>6</sub>N<sub>4</sub>, bpym),  $\mu$ -oxalato-bridged (C<sub>2</sub>O<sub>4</sub><sup>2-</sup>, ox) and  $\mu$ -chloro-bridged Cu(II) network [Cu<sub>2</sub>(bpym)(ox)Cl<sub>2</sub>]<sub>n</sub> is reported. The compound crystallizes in the orthorhombic system, space group Pbca, with a 9.522(2), b 10.509(2), c 13.222(3) Å, Z = 4. The structure consists of alternately  $\mu$ -bpym- and  $\mu$ -ox bridged Cu(II) chains which again are connected through mono( $\mu$ -chloro) ligands, thus forming a corrugated two-dimensional (2D) framework. Polarized optical single crystal absorption spectra, measured at both room and liquid-He temps., are presented and the absorption pattern is discussed using the selection rules derived from an orbital scheme of the Cu(II) chromophore with idealized C<sub>2v</sub> symmetry. A low-lying MLCT state is taken as the origin of the strongly polarized absorption parallel to the b-axis, hence the ox-Cu(II)-bpym direction. The temperature dependence of the magnetic susceptibility is well explained with an alternating chain model, taking into account the strong intramol. antiferromagnetic interaction through the  $\mu$ -bpym and  $\mu$ -ox bridges. The exchange parameters are J = -189(1) cm<sup>-1</sup> for the  $\mu$ -ox link and  $\alpha$ J = -76(1) cm<sup>-1</sup> for the  $\mu$ -bpym link, which corresponds to an alternation parameter of  $\alpha$  0.40(2). A mean-field correction is discussed which considers the possibility of weak interchain interactions mediated by the asym. mono( $\mu$ -chloro) bridges.

L5 ANSWER 41 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:817836 CAPLUS  
 DN 123:245263  
 TI An oxalate-linked copper(II) coordination polymer, [Cu<sub>2</sub>(oxalate)<sub>2</sub>(pyrazine)<sub>3</sub>]<sub>n</sub>, constructed with two different copper units: x-ray crystallographic and electronic structures  
 AU Kitagawa, Susumu; Okubo, Takashi; Kawata, Satoshi; Kondo, Mitsuru; Katada, Motomi; Kobayashi, Hisayoshi  
 CS Dep. of Chem., Tokyo Metropolitan Univ., Tokyo, Japan  
 SO Inorganic Chemistry (1995), 34(19), 4790-6  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB The new Cu(II) coordination polymer [Cu<sub>2</sub>( $\mu$ -ox)<sub>2</sub>( $\mu$ -pyz)(pyz)<sub>2</sub>]<sub>n</sub> (1) (ox = oxalate; pyz = pyrazine) was synthesized and characterized. 1 Crystallizes in the triclinic space group P<sub>1</sub>h<sub>1</sub> with a 10.578(4)Å, b 11.603(5) Å, c 8.027(4) Å,  $\alpha$  92.11(5),  $\beta$  103.10(3),

$\gamma$  76.32(4)°,  $Z = 2$ , and chemical formula  $\text{Cu}_2\text{C}_{16}\text{N}_6\text{O}_8\text{H}_{12}$ . 1 Shows an extended sheet structure of Cu(II) ions bridged by oxalate anions and pyrazine. The repeating unit of  $(\text{Cu}_2(\mu\text{-ox})_2(\mu\text{-pyz})(\text{pyz})_2)$  contains two types of 4 + 2 coordination environments with  $\text{O}_4\text{N}_2$ , which are characteristic of pyz coordination; one of the two Cu atoms has only terminally coordinated pyz mols. while the other is linked by bridging pyz mols. The Cu-ox-Cu-sequence displays as pleated ribbon, thus planes of Cu-ox-Cu form a boat conformation. In addition to the coordination bond linking, there is stack linking of pyz mols. whose column runs along the ribbon. The magnetic susceptibilities were measured to 2 K and analyzed in terms of an alternating-chain Heisenberg-exchange model ( $H = -2J\sum_i \mathbf{S}_{2i} \cdot \mathbf{S}_{2i-1} + \alpha \mathbf{S}_{2i} \cdot \mathbf{S}_{2i+1}$ ) to yield  $J = -20.4 \text{ cm}^{-1}$  and  $\alpha = 0.85$ . The alternate arrangement of the Cu geometries along a ribbon leads to that of the magnetic orbitals. This well explains the value of  $J$  smaller than that of  $[\text{Cu}(\text{ox})]_n$  without apical ligands and comparable to that of  $[\text{Cu}(\text{ox})(\text{NH}_3)_2]_n$ . The d. functional MO calcn. and EHMO band calcns. were carried out to delineate the electronic structure and the role of pyz mols. in the extended structure.

L5 ANSWER 42 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:559620 CAPLUS

DN 123:46698

TI Synthesis and structure study of the complex  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2](\text{C}_6\text{H}_4\text{COSO}_2\text{N})_2$ . Crystal structure containing Cu(II) bipy oxalato and saccharin

AU Jianmin, Li; Jingzhen, Sun; Pengcheng, Chen; Xintao, Wu

CS Dep. Modern Chem., Univ. Sci. Technol. China, Hefei, Peop. Rep. China

SO Crystal Research and Technology (1995), 30(3), 353-8

CODEN: CRTEDF; ISSN: 0232-1300

PB Akademie Verlag

DT Journal

LA English

AB  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{bipy})_2(\text{H}_2\text{O})_2](\text{C}_6\text{H}_4\text{COSO}_2\text{N})_2$  ( $\text{C}_6\text{H}_4\text{COSO}_2\text{N}$  = saccharin anion) was synthesized and its crystal structure determined at room temperature  $MW = 927.86$ , monoclinic, space group  $P2_1/c$ ,  $Z = 2$ ,  $a$  9.283(1),  $b$  16.239(2),  $c$  12.209(1) Å,  $\beta$  99.848(9)°. The crystal structure consists of repeated  $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]_2$  cations and noncoordinated saccharin anions. Each Cu ion is in a square pyramidal environment with two oxalate O and two bipyridine N atoms as a base and one  $\text{H}_2\text{O}$  mol. at the apex. The two Cu ions are bridged by oxalate and the distance is 5.138 Å.

L5 ANSWER 43 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:393360 CAPLUS

DN 122:175077

TI Crystal structure of  $\mu$ -oxalato-bis[di-(2-aminoethyl)aminecopper(II)] diperchlorate monohydrate,  $(\text{C}_4\text{H}_{13}\text{N}_3\text{Cu})_2(\text{C}_2\text{O}_4)(\text{ClO}_4)_2 \cdot \text{H}_2\text{O}$

AU Kruger, P. E.; Murray, K. S.; Tiekink, E. R. T.

CS Dep. Chem., Monash Univ., Clayton, 3168, Australia

SO Zeitschrift fuer Kristallographie (1994), 209(7), 624-5

CODEN: ZEKRDZ; ISSN: 0044-2968

PB Oldenbourg

DT Journal

LA English

AB The title compound is orthorhombic, space group  $Pbcm$ , with  $a$  6.877(5),  $b$  13.045(5),  $c$  24.855(5) Å;  $Z = 4$ ,  $R = 0.053$ ,  $R_w = 0.063$ . Atomic coordinates are given. The title compound is centrosym. and crystallizes as a hydrate such that for every 2 Cu atoms there is 1  $\text{H}_2\text{O}$  mol. of crystallization. The unhydrated form crystallizes in a noncentric space group.

L5 ANSWER 44 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:327238 CAPLUS

DN 122:150119

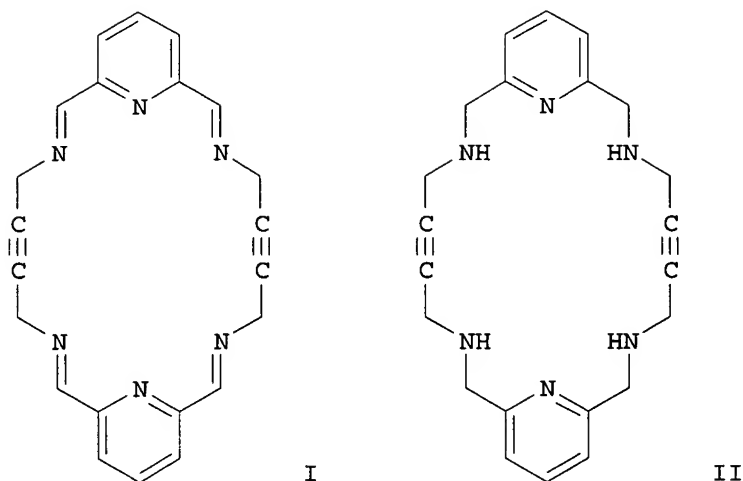
TI Synthesis and structure of dinuclear copper(II) complexes of a novel hexaaza macrocycle containing bridging oxalate and acetate ions

AU Warzeska, Sabine; Kraemer, Roland

CS Anorganisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany

SO Chemische Berichte (1995), 128(2), 115-19

PB VCH  
 DT Journal  
 LA German  
 GI



AB Nontemplate Schiff base [2 + 2] condensation of pyridine-2,6-dicarbaldehyde with 1,4-diamino-2-butyne yields I, which is converted to II by NaBH<sub>4</sub> reduction of the amino groups. [(II)Cu<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)](BPh<sub>4</sub>)<sub>2</sub> (3) and [(II)Cu<sub>2</sub>(μ-AcO)(OH<sub>2</sub>)](PF<sub>6</sub>)<sub>2</sub>·2.25(NO<sub>3</sub>)<sub>0.75</sub> (4), were characterized by x-ray crystallog. The oxalate ligand in 3 forms a (μ-η<sup>4</sup>:η<sup>4</sup>) bridge between the Cu atoms. 4 Contains a syn-anti-bridging acetate ion. The Cu-Cu distances are 5.315 Å in 3 and 3.746 Å in 4, resp. Oxalate can be separated from other carboxylates in aqueous solution by selective binding to the [(II)Cu<sub>2</sub>] unit and precipitation of 3.

L5 ANSWER 45 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:259419 CAPLUS

DN 120:259419

TI Very High-Field Magnetization and Intermolecular Interactions: Application to {[tmen(2-MeIm)Cu]<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)}(PF<sub>6</sub>)<sub>2</sub> (tmen = N,N,N',N'-Tetramethylethylenediamine, 2-MeIm = 2-Methylimidazole)

AU Bergerat, Pierre; Kahn, Olivier; Legoll, Patrick; Drillon, Marc; Guillot, Maurice

CS Laboratoire de Chimie Inorganique, Universite de Paris Sud, Orsay, 91405, Fr.

SO Inorganic Chemistry (1994), 33(9), 2049-51

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Some years ago the crystal structure and the magnetic properties of {[tmen(2-Melm)Cu]<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)}(PF<sub>6</sub>)<sub>2</sub> (tmen = N,N,N',N'-tetramethylethylenediamine, 2-Melm = 2-methylimidazole) had been reported. The structure consists of centrosym. oxalatobridged copper(II) binuclear units and PF<sub>6</sub> anions. The temperature dependence of the magnetic susceptibility had been interpreted as resulting from an antiferromagnetic intramol. interaction. No intermol. effect had been taken into account. The field dependence of the magnetization up to 200 kOe was measured at 3 and 4.2 K. The exptl. data do not follow at all the theor. behavior expected in a purely mol. model. Actually, these very high-field magnetization data reveal that the intermol. interactions play an important role. A careful examination of the crystal structure showed that the binuclear units are hydrogen bonded, forming a sort of chain of binuclear units. A theor. model for the magnetization taking into account this topol. was elaborated. Least-squares fitting of the susceptibility and magnetization data led to a ratio J'/J between inter- and intramol. interaction

parameters equal to 0.4. The compound has a significant 1-dimensional character, which could not be anticipated from magnetic susceptibility data. Only high-field magnetization measurements could provide this information.

- L5 ANSWER 46 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1994:151723 CAPLUS  
DN 120:151723  
TI Magnetic properties of the dinuclear copper(II) compounds bridged by oxalato-type ligands  
AU Emori, Shuji; Todoko, Kyoto  
CS Fac. Sci. Eng., Saga Univ., Saga, 840, Japan  
SO Bulletin of the Chemical Society of Japan (1993), 66(11), 3513-15  
CODEN: BCSJA8; ISSN: 0009-2673  
DT Journal  
LA English  
AB Various dinuclear copper(II) compds. bridged by the oxalato, oxamato, and oxamidato ligands were prepared and characterized by magnetic susceptibility and IR spectroscopy. The strong antiferromagnetic couplings through their carboxylate or carboxamate groups are interpreted in terms of the ligand basicities and the electron withdrawal due to the resonance of the substituents.
- L5 ANSWER 47 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1993:481271 CAPLUS  
DN 119:81271  
TI Thermodynamics of coordination of metal ions with binucleating macrocyclic and macrobicyclic ligands  
AU Martell, Arthur E.; Motekaitis, Ramunas J.; Chen, Dian; Murase, Ichiro  
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843-3255, USA  
SO Pure and Applied Chemistry (1993), 65(5), 959-64  
CODEN: PACHAS; ISSN: 0033-4545  
DT Journal  
LA English  
AB The stabilities of the Cu(II) complexes of binucleating macrocyclic and macrobicyclic ligands, and the equilibrium consts. with bridging anions for the Cu(II) and Co(II) complexes formed by these ligands, are described. The binuclear Co(II) dioxygen complexes are present as examples of a bridging anion coordinated simultaneously to 2 metal centers.
- L5 ANSWER 48 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1993:138530 CAPLUS  
DN 118:138530  
TI Two different (oxalato)(bipyridine)copper(II) complexes in one single crystal. Crystal structures and magnetic properties of [Cu<sub>2</sub>(bipy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]X<sub>2</sub>. [Cu(bipy)(C<sub>2</sub>O<sub>4</sub>)] (X = NO<sub>3</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup> or ClO<sub>4</sub><sup>-</sup>)  
AU Gleizes, Alain; Julve, Miguel; Verdaguer, Michel; Real, Jose Antonio; Faus, Juan; Solans, Xavier  
CS Cent. Elaboration Mater. Etud. Struct., Univ. Paul Sabatier, Toulouse, 31055, Fr.  
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1992), (22), 3209-16  
CODEN: JCDTBI; ISSN: 0300-9246  
DT Journal  
LA English  
AB [Cu<sub>2</sub>(bpy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]X<sub>2</sub>. [Cu(bpy)(C<sub>2</sub>O<sub>4</sub>)] (1-3; bpy = 2,2'-bipyridine; H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> = oxalic acid, X = NO<sub>3</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup>, ClO<sub>4</sub><sup>-</sup>) were prepared and their crystal structures determined by single-crystal x-ray diffraction methods at room temperature. They are all isostructural and crystallize in the monoclinic system, space group C2/c, Z = 4; final R (R') = 0.029 (0.051) for 1, 0.033 (0.046) for 2 and 0.057 (0.059) for 3. Their structures consist of cationic centrosym. dinuclear [Cu<sub>2</sub>(bpy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]<sup>2+</sup> units, neutral axiosym. mononuclear [Cu(bpy)(C<sub>2</sub>O<sub>4</sub>)] entities and either NO<sub>3</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup> or ClO<sub>4</sub><sup>-</sup> as counterion. Each Cu atom of the dinuclear species is in a square-pyramidal environment with 2 oxalate O and 2 bipyridine N atoms as a base and a H<sub>2</sub>O mol. at the apical position. The Cu atom of the mononuclear complex is in a slightly tetrahedrally distorted square comprised of 2 bipyridine N and 2 oxalate O atoms. In both complexes 1 or 2 more distant atoms of the counterion

completes a (5 + 1) or a (4 + 2) Cu coordination, resp. The mono- and di-nuclear entities form an alternating chain via weak interactions through counterions and Cu atoms. Variable-temperature (20-300 K) magnetic susceptibility measurements revealed a strong antiferromagnetic interaction within the dinuclear unit, the singlet-triplet energy gap being -386, -378 and -376 cm<sup>-1</sup>, resp. The  $\chi_{MT}$  vs. T curve for all 3 complexes exhibits a plateau at T < 80 K which corresponds to the Curie law expected for the mononuclear complex. The magnitude of the exchange coupling in this series was analyzed in the framework of a simple orbital model.

L5 ANSWER 49 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:206624 CAPLUS

DN 116:206624

TI A new synthetic route for polynuclear oxalato adducts

AU Gueye, Omar; Diop, Libasse

CS Fac. Sci., Univ. C.A. Diop, Dakar, Senegal

SO Bulletin of the Chemical Society of Ethiopia (1991), 5(2), 103-6

CODEN: BCETE6; ISSN: 1011-3924

DT Journal

LA English

AB (MX<sub>2</sub>)<sub>2</sub>(Me<sub>4</sub>N)<sub>2</sub>C<sub>2</sub>O<sub>4</sub>.nH<sub>2</sub>O (M = Cd, Cu, Co, Mn, X = Cl; M = Cu, Cd, X = Br), (SbCl<sub>3</sub>)<sub>2</sub>(Me<sub>4</sub>N)<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, (BiCl<sub>3</sub>)<sub>2</sub>(Me<sub>4</sub>N)<sub>2</sub>C<sub>2</sub>O<sub>4</sub> and (HgCl<sub>2</sub>)<sub>4</sub>(Me<sub>4</sub>N)<sub>2</sub>C<sub>2</sub>O<sub>4</sub> were prepd from the resp. metal halides and (Me<sub>4</sub>N)<sub>2</sub>C<sub>2</sub>O<sub>4</sub>. The structures were established on the basis of IR data.

L5 ANSWER 50 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:96365 CAPLUS

DN 116:96365

TI Structure of ( $\mu$ -oxalato)-trans-bis[(N,N,N',N'-tetramethylethylenediamine)perfluoro-tert-butoxycopper(II)]benzene solvate

AU George, Clifford; Purdy, Andrew

CS Lab. Struct. Matter, Nav. Res. Lab., Washington, DC, 20375, USA

SO Acta Crystallographica, Section C: Crystal Structure Communications (1992), C48(1), 155-7

CODEN: ACSCEE; ISSN: 0108-2701

DT Journal

LA English

AB The title compound is monoclinic, space group C2/m, with a 14.581(5), b 12.484(4), c 13.239(5) Å, and  $\beta$  123.05(2)°; Z = 2,  $d_c$  = 1.637, final R = 0.055,  $R_w$  = 0.067 for 1629 reflections. Atomic coordinates are given. The distorted square-pyramidal 5-coordinate CuII complex and the benzene solvate both have C<sub>2h</sub> mol. symmetry. The asym. unit consists of 1/4 of the Cu complex and 1/4 of the solvate mol. All of the CF<sub>3</sub> groups are poorly defined and the fluorines of one of the crystallog. independent CF<sub>3</sub> groups were treated as a disorder with occupancies of 52 and 48% resp.

L5 ANSWER 51 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:669241 CAPLUS

DN 115:269241

TI Crystal and molecular structure and magnetic properties of a new  $\mu$ -oxalato binuclear copper(II) complex containing mepirizole

AU Soto Tuero, Lucia; Garcia-Lozano, Julia; Escrivá Monto, Emilio; Beneto Borja, Matilde; Dahan, Francoise; Tuchagues, Jean Pierre; Legros, Jean Pierre

CS Fac. Farm., Univ. Valencia, Valencia, 46010, Spain

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1991), (10), 2619-24

CODEN: JC DTBI; ISSN: 0300-9246

DT Journal

LA English

AB The preparation and crystal and mol. structure are reported of [(mpym)(H<sub>2</sub>O)(NO<sub>3</sub>)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(NO<sub>3</sub>)(H<sub>2</sub>O)(mpym)].2H<sub>2</sub>O (mpym = mepirizole). Crystals are monoclinic, space group P2, a 7.559(4), b 14.659(3), c 16.246(3) Å,  $\beta$  98.6(2)°, Z = 2, R = 0.046,  $R'$  = 0.047. It consists of discrete binuclear entities where the Cu atoms lie in a strongly elongated octahedral environment, surrounded by 2 N atoms (1 from each ring of a mepirizole mol.) and 2 O atoms of the bridging C<sub>2</sub>O<sub>4</sub><sup>2-</sup> group

in the equatorial plane and O atoms of H<sub>2</sub>O mols. and NO<sub>3</sub><sup>-</sup> in the axial positions. The binuclear entities are not centrosym. and the difference in the ligand environments of the Cu(II) ions induces an energy separation between the 2 magnetic orbitals large enough to weaken the antiferromagnetic interaction ( $J = -142 \text{ cm}^{-1}$ ) by .apprx.60  $\text{cm}^{-1}$  compared to that of sym.  $\mu$ -oxalato binuclear Cu(II) compds. ESR, vibrational and electronic spectra are consistent with the above results.

L5 ANSWER 52 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:646618 CAPLUS

DN 115:246618

TI Complex formation between oxalate and (2,2':6',2''-terpyridyl)copper(II) in dimethyl sulfoxide solution. Synthesis and crystal structures of mono- and dinuclear complexes

AU Castro, Isabel; Faus, Juan; Julve, Miguel; Gleizes, Alain

CS Fac. Quim., Univ. Valencia, Burjassot, 46100, Spain

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1991), (8), 1937-44

CODEN: JCDTBI; ISSN: 0300-9246

DT Journal

LA English

AB The crystal and mol. structures of new  $[\{\text{Cu}(\text{terpy})(\text{H}_2\text{O})\}_2(\text{ox})][\{\text{Cu}(\text{terpy})\}_2(\text{ox})][\text{ClO}_4] \cdot 4.2\text{H}_2\text{O}$  (I) and  $[\text{Cu}(\text{terpy})(\text{H}_2\text{O})(\text{ox})] \cdot 4\text{H}_2\text{O}$  (II; terpy = 2,2':6',2''-terpyridine, H<sub>2</sub>ox = oxalic acid) were determined by X-ray diffraction. Crystals of I are monoclinic, space group P2<sub>1</sub>/c,  $a = 13.443(2)$ ,  $b = 23.183(4)$ ,  $c = 12.394(1) \text{ \AA}$ ,  $\beta = 116.29(1)^\circ$ ,  $Z = 2$ ,  $R = 0.045$ ,  $R' = 0.063$ ; those of II are triclinic, space group P<sub>1</sub>h<sub>1</sub>in.1,  $a = 10.192(1)$ ,  $b = 12.319(2)$ ,  $c = 8.397(3) \text{ \AA}$ ,  $\alpha = 86.65(3)$ ,  $\beta = 96.80(3)$ , and  $\gamma = 106.14(1)^\circ$ ,  $Z = 2$ ,  $R = 0.044$ ,  $R' = 0.052$ . The structure of I contains 2 different centrosym. Cu(II) dinuclear dicationic units, uncoordinated ClO<sub>4</sub><sup>-</sup> groups and lattice H<sub>2</sub>O. In both dinuclear units the terpyridyl group is terminal and the oxalate acts as an asym. bis(chelating) bridge. The Cu atom is 5-coordinate in 1 dinuclear unit and 6-coordinate in the other. The structure of II consists of  $[\text{Cu}(\text{terpy})(\text{H}_2\text{O})(\text{ox})]$  entities and uncoordinated H<sub>2</sub>O mols. The Cu atom is in a 6-coordinate, tetragonally elongated, octahedral environment. The stability consts.  $[\text{Cu}(\text{terpy})]^{2+} + \text{ox}^{2-} + \text{H}^+ \text{ .dblharw. } [\text{Cu}(\text{terpy})(\text{Hox})]^+; 2[\text{Cu}(\text{terpy})]^{2+} + \text{ox}^{2-} \text{ .dblharw. } [\{\text{Cu}(\text{terpy})\}_2(\text{ox})]^{2+};$  and  $[\text{Cu}(\text{terpy})]^{2+} + \text{ox}^{2-} \text{ .dblharw. } [\text{Cu}(\text{terpy})(\text{ox})]$  were determined by potentiometry in DMSO solution:  $\log \beta = 12.397(4)$ ,  $10.621(6)$ , and  $7.394(2)$ , resp. ( $25^\circ$  0.1 mol dm<sup>-3</sup> [NBu<sub>4</sub>][ClO<sub>4</sub>]). The coordination modes of oxalate in the CuIIL-ox<sup>2-</sup> system (L being tri- or bi-dentate N-donor ligands) are discussed in the light of available thermodyn. and structural parameters.

L5 ANSWER 53 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:440757 CAPLUS

DN 115:40757

TI Structure of the first polymeric catena- $\mu$ -tris[oxalato(2-)-O1,O2; O3,O4]dicopper complex with interlocked helical chains

AU Sundberg, Markku R.; Kivekas, Raikko; Koskimies, Jorma K.

CS Div. Inorg. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland

SO Journal of the Chemical Society, Chemical Communications (1991), (7), 526-7

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

AB Oxidation of a mixture of Cu(II), vitamin C, and Et<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>OH in the presence of H<sub>2</sub>O<sub>2</sub> yielded a polymeric catena- $[\text{Cu}_2(\mu\text{-C}_2\text{O}_4)_3]^{2-}$  with CuII surrounded by 6 O atoms of 3 C<sub>2</sub>O<sub>4</sub><sup>2-</sup> ions, each one starting a helical chain. Crystal data: monoclinic, space group C2/c,  $a = 14.297(3)$ ,  $b = 10.472(2)$ ,  $c = 18.539(3) \text{ \AA}$ ,  $\beta = 114.068(13)^\circ$ ,  $Z = 8$ ,  $R = 0.051$ ,  $R_w = 0.047$ .

L5 ANSWER 54 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:420881 CAPLUS

DN 115:20881

TI Study of the interaction between 2,2'-bipyridinecopper(2+) and oxalate in dimethyl sulfoxide. Crystal structure of  $[\text{Cu}_2(\text{bipy})_2(\text{H}_2\text{O})_2(\text{ox})]\text{SO}_4 \cdot [\text{Cu}(\text{bipy})$



)ox]  
 AU Castro, Isabel; Faus, Juan; Julve, Miguel; Munoz, M. Carmen; Diaz,  
 Wladimiro; Solans, Xavier  
 CS Fac. Quim., Univ. Valencia, Burjassot, 46100, Spain  
 SO Inorganica Chimica Acta (1991), 179(1), 59-66  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 AB A study of complex formation between  $[\text{Cu}(\text{bipy})]^{2+}$  and  $\text{ox}^{2-}$  (bipy =  
 2,2'-bipyridine;  $\text{H}_2\text{ox}$  = oxalic acid), was carried out by potentiometry in  
 DMSO solution. The consts. of the equilibrium  $[\text{Cu}(\text{bipy})]^{2+} + \text{ox}^{2-} \rightleftharpoons$   
 $[\text{Cu}(\text{bipy})\text{ox}]$  (1) and  $2[\text{Cu}(\text{bipy})]^{2+} + \text{ox}^{2-} \rightleftharpoons [\text{Cu}_2(\text{bipy})_2\text{ox}]^{2+}$  (2)  
 are  $\log \beta_2 = 13.185(5)$  at  $25^\circ$  and  $0.1 \text{ mol dm}^{-3} \text{ Bu}_4\text{NClO}_4$ . The  
 high values of these consts. are consistent with the sym. bidentate and  
 bis-bidentate modes of oxalate in  $[\text{Cu}(\text{bipy})\text{ox}]$  and  $[\text{Cu}_2(\text{bipy})_2\text{ox}]^{2+}$  units,  
 resp., as shown by x-ray diffraction studies. Single crystals of  
 $[\text{Cu}_2(\text{bipy})_2(\text{H}_2\text{O})_2\text{ox}]\text{SO}_4 \cdot [\text{Cu}(\text{bipy})\text{ox}]$  (I) were grown from aqueous solns. and  
 characterized by x-ray diffraction. I is monoclinic, space group  $\text{C}2/c$ ,  $a$   
 $22.706(5)$ ,  $b$   $10.485(3)$ ,  $c$   $16.172(4) \text{ \AA}$ ,  $\beta$   $92.63(3)^\circ$ ,  $Z = 4$ ,  
 $R = 0.067$ ,  $R_w = 0.070$ . The structure is made up of cationic centrosym.  
 $[\text{Cu}_2(\text{bipy})_2\text{ox}]^{2+}$  dinuclear units, neutral axial-sym.  $[\text{Cu}(\text{bipy})\text{ox}]$   
 mononuclear entities, and  $\text{SO}_4^{2-}$  as a counterion. Each Cu atom of the  
 dinuclear unit shows a square-pyramidal environment with the 2 N atoms of  
 bipy and 2 O atoms of oxalato bridge building the basal plane and an O  
 atom of a  $\text{N}_2\text{O}$  mol. filling the apical position. The Cu atom of the  
 mononuclear unit is bound to 2 O atoms of oxalate and 2 N atoms of bipy  
 forming a 4-fold surrounding slightly deviating from planarity. In these  
 complexes, Cu coordination is  $4 + 1 + 1$  (dinuclear unit) or  $4 + 2$   
 (mononuclear unit) because of the weak binding of the group in a  
 bis-monodentate fashion linking alternately dinuclear and mononuclear  
 entities. This is a rare case where the 2 Cu(II) complexes bound to the  
 same ligands, that have been observed in solution, are found in the same compound  
 in the solid state.

L5 ANSWER 55 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:603759 CAPLUS

DN 113:203759

TI Binuclear copper(II) complexes of 1,4,7-trimethyl-1,4,7-triazacyclononane:  
 synthesis, spectroscopy, and spin coupling across multiple-atom bridges of  
 variable length (3.6-7.6  $\text{\AA}$ )

AU Chaudhuri, Phalguni; Oder, Karen

CS Ruhr-Univ., Bochum, D-4630/1, Germany

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry  
 (1972-1999) (1990), (5), 1597-605

CODEN: JCDTBI; ISSN: 0300-9246

DT Journal

LA English

AB Thirteen  $[\text{LCu}(\mu\text{-X})\text{CuL}]^{2+}$  ( $\text{L} = 1,4,7\text{-trimethyl-1,4,7-triazacyclononane}$ ;  
 $\text{X} = \text{Cl}, \text{Br}, \text{SCN}, 0.5\text{C}_2\text{O}_4, 0.5 \text{ oxamato}, 0.5 \text{ 2,5-dichlorobenzene-1,3,4,6-}$   
 $\text{tetrahydroxo}, 0.5 \text{ benzene-1,2,4,5-tetrahydroxo}, \text{ and } \text{AcO-}$ ) were synthesized  
 and characterized based on IR, electronic, and ESR spectroscopy and  
 variable-temperature (100-300 K) magnetic susceptibility measurements. A  
 varying range of magnetic interactions, no coupling, antiferromagnetic ( $2J$   
 $= -460 \text{ cm}^{-1}$ ), and ferromagnetic ( $J = +22 \text{ cm}^{-1}$ ) coupling, was observed between  
 the Cu(II) ions in these binuclear systems with variable metal-metal separation  
 estimated 3.6-7.6  $\text{\AA}$ . The interaction is more effective through a  
 $\mu\text{-oxamato}$  bridge ( $2J = -460 \text{ cm}^{-1}$ ) than through a  $\mu\text{-oxalato}$  bridge  
 ( $2J = -300 \text{ cm}^{-1}$ ). A moderately strong antiferromagnetic interaction ( $2J =$   
 $-60 \text{ cm}^{-1}$ ) was found for the 2,5-dichlorobenzene-1,3,4,6-tetrahydroxo-  
 bridged compound, where the Cu...Cu separation is expected to be  $\text{apprx.} 7.6$   
 $\text{\AA}$ . The X-band ESR spectra of the polycryst. substances at 120 K  
 indicate square-pyramidal geometry for the Cu with a  $(dx^2-y^2)_1$  ground  
 state. A mixed bridged compound ( $\mu\text{-1,1-N}_3$ )( $\mu\text{-OH}$ ), with a  
 ferromagnetic interaction between the Cu centers is described. The  
 difference in magnetic exchange interaction between the different Cu(II)  
 systems is discussed.

L5 ANSWER 56 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1990:598432 CAPLUS

DN 113:198432  
 TI Oxalato-bridged and related dinuclear copper(II) complexes: theoretical analysis of their structures and magnetic coupling  
 AU Alvarez, Santiago; Julve, Miguel; Verdaguer, Michel  
 CS Dep. Quim. Inorg., Univ. Barcelona, Barcelona, 08028, Spain  
 SO Inorganic Chemistry (1990), 29(22), 4500-7  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB A theor. anal. is given of the structural variations found for dinuclear Cu(II) complexes with oxalato and related polynuclear bridging ligands and their influence on the magnitude of the magnetic exchange interactions. The family of compds. studied can be represented by the general formula  $[(AA)Cu(\mu-C_2O_4)Cu(AA)]X_n$ , where AA can be a chelating ligand like 2,2'-bipyridine (bpy) or tetramethylethylenediamine (tmen), and X is a counteranion or a solvent mol. Three types of distortions from an ideal square-planar geometry around the Cu atoms are considered: (1) the removal of the Cu ions from the ligands' plane; (2) a twist of the square planar  $A_2CuO_2$  cores toward a tetrahedral geometry by rotation of the AA ligand; (3) folding of the  $A_2Cu-ox-CuA_2$  skeleton through the O--O hinges and the axial coordination of X. An evaluation of the second-order Jahn-Teller distortions through the anal. of orbital topologies and the atomic electronegativities is presented, which might be helpful in predicting how stable a distorted mol. is relative to the undistorted one, as well as the relative extent for such distortions in a series of related structures.

L5 ANSWER 57 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1990:110667 CAPLUS  
 DN 112:110667  
 TI Formation in solution, synthesis and crystal structure of  $\mu$ -oxalatobis[bis(2-pyridylcarbonyl)amido]dicopper(II)  
 AU Castro, Isabel; Faus, Juan; Julve, Miguel; Mollar, Miquel; Monge, Angeles; Gutierrez-Puebla, Enrique  
 CS Fac. Cienc. Quim., Univ. Valencia, Burjassot, 46100, Spain  
 SO Inorganica Chimica Acta (1989), 161(1), 97-104  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 AB  $[Cu_2L_2(C_2O_4)]$  (HL = bis(2-pyridylcarbonyl)amide) was synthesized and characterized by spectroscopy, ESR and diffraction methods. It crystallizes in the triclinic space group  $P_{\bar{1}}$ ,  $a$  7.6793(6),  $b$  9.238(2),  $c$  10.007(2) Å,  $\alpha$  83.80(1),  $\beta$  68.37(1) and  $\gamma$  69.44(1)°,  $Z$  = 2,  $d_c$  = 1.80 g cm<sup>-3</sup>, for 2391 with  $I \geq 2\sigma(I)$   $R$  and  $R_w$  0.049 and 0.053, resp. The structure consists of neutral centrosym. binuclear entities in which  $C_2O_4^{2-}$  acts in an asym. bis-bidentate fashion. Each Cu atom is in a square-pyramidal environment with the 3 N atoms of bis(2-pyridylcarbonyl)amido anion and an O atom of oxalate in the basal plane and another O atom of oxalate occupying the apical position. The stability consts. of the  $Cu-L-C_2O_4^{2-}$  complexes were determined in DMSO solution. Coordination modes of oxalate for this system are compared in DMSO and water in the light of thermodyn. and structural parameters.

L5 ANSWER 58 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1989:508023 CAPLUS  
 DN 111:108023  
 TI Synthesis, characterization and magnetic properties of  $\mu$ -oxalato- and  $\mu$ -oxamido-bridged copper(II) dimers. Crystal and molecular structures of  $[Cu_2(mepirizole)_2(C_2O_4)(H_2O)_2](PF_6)_2 \cdot mepirizole \cdot 3H_2O$  and  $[Cu_2(mepirizole)_2(C_2O_4)(NO_3)_2(H_2O)]_2[Cu_2(mepirizole)_2(C_2O_4)(NO_3)_2]$   
 AU Soto, L.; Garcia, J.; Escriva, E.; Legros, J. P.; Tuchagues, J. P.; Dahan, F.; Fuertes, A.  
 CS Dep. Quim. Inorg., Univ. Valencia, Valencia, 46010, Spain  
 SO Inorganic Chemistry (1989), 28(17), 3378-86  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB  $[Cu_2L_2(C_2O_4)(H_2O)_2](PF_6)_2 \cdot L \cdot 3H_2O$  (I),  $[Cu_2L_2(C_2O_4)(NO_3)_2(H_2O)]_2/[Cu_2L_2(C_2O_4)(NO_3)_2]$  (II),  $Cu_2L_2(C_2O_4)(ClO_4)_2$ , and  $Cu_2L_2(oxamd)(NO_3)_2 \cdot H_2O$ ,  $H$  = oxamd

= oxamine, and L = mepirizole (4-methoxy-2-(5-methoxy-3-methyl-pyrazol-1-yl)-6-methylpyrimidine)] were prepared. The structures of I and II were determined, I crystallizes in the orthorhombic system, space group Pnma, with  $Z = 8$ . II crystallizes in the monoclinic system, space group P2<sub>1</sub>/n, with  $Z = 4$ . The structure of I consists of centrosym. binuclear cations  $[L(H_2O)Cu(C_2O_4)Cu(H_2O)L]^{2+}$  separated by PF<sub>6</sub><sup>-</sup> anions and mols. of free mepirizole and water of crystallization. The structure of II is composed of 2 crystallog. independent dimers  $[L(NO_3)Cu(C_2O_4)Cu(NO_3)(H_2O)L]$  and  $[L(NO_3)Cu(C_2O_4)Cu(NO_3)L]$ . The 4 complexes were studied with IR, UV-visible, and ESR spectroscopies and magnetic susceptibility measurements at 360-5 K. The 4 complexes exhibit strong antiferromagnetic exchange interactions ranging from -156 to -201 cm<sup>-1</sup>. Magnetic and ESR results are discussed with respect to the crystal structures of I and II.

L5 ANSWER 59 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1989:507975 CAPLUS  
 DN 111:107975  
 TI Magnetic properties of mono-, bi-, and tri-nuclear copper(II) complexes of novel oxamato and oxamido ligands. Crystal structure of a mononuclear precursor  
 AU Costes, Jean Pierre; Dahan, Francoise; Laurent, Jean Pierre  
 CS Lab. Chim. Coord., CNRS, Toulouse, 31077, Fr.  
 SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1989), (6), 1017-25  
 CODEN: JCDBTBI; ISSN: 0300-9246  
 DT Journal  
 LA English  
 AB MeC(O)CH:C(Me)NHCH<sub>2</sub>CH<sub>2</sub>NC(O)C(O)R (H<sub>3</sub>L; R = OH, NH<sub>2</sub>, NHMe) were prepared and used to prepare  $[CuL] \cdot Na[CuL(H_2O)] \cdot 0.33H_2O$  (R = OH) crystallizes in the monoclinic system, space group P2<sub>1</sub>/n, with a 21.705(2), b 9.380(1), c 19.131(2) Å, and  $\beta$  110.17(1)°. The structure consists of 3 mononuclear anions  $[CuL]^-$  together with 3 Na cations and 4 H<sub>2</sub>O mols. From the mononuclear fragments, binuclear complexes  $[CuLCuL_1]^+$  (L<sub>1</sub> = 2,2'-bipyridine or diethylenetriamine) were prepared and spectroscopically characterized.  $[Cu_2L_2]$  [H<sub>4</sub>L<sub>2</sub> = N,N'-bis(4-methyl-6-oxo-3-azahept-4-enyl)oxamide],  $[(CuL)_2Cu]$  (R = OH) and  $[(CuL)_2Zn]$  (R = OH) were prepared. The magnetic properties of these complexes were studied at 5-290 K. The importance of the antiferromagnetic interactions mediated by the oxamato and oxamido bridges is discussed with respect to the nature of the HL and L<sub>1</sub> ligands.

L5 ANSWER 60 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1988:197232 CAPLUS  
 DN 108:197232  
 TI Synthesis and spectral studies of N-2-pyridinylcarbonyl-2-pyridinecarboximate copper(II) complexes  
 AU Folgado, Jose V.; Escrivá, Emilio; Beltrán-Porter, Aurelio; Beltrán-Porter, Daniel  
 CS Dep. Quim. Inorg., Univ. Valencia, Valencia, 46100, Spain  
 SO Transition Metal Chemistry (Dordrecht, Netherlands) (1987), 12(4), 306-10  
 CODEN: TMCHDN; ISSN: 0340-4285  
 DT Journal  
 LA English  
 AB Cu(BPCA)X.nH<sub>2</sub>O [X = Cl, Br, NCS, NCO, N<sub>3</sub>, or CN] and Cu<sub>2</sub>(BPCA)2X.nH<sub>2</sub>O [H<sub>2</sub>X = oxalic acid, chloranilic acid or 2,5-dihydroxy-1,4-benzoquinone; HBPCA = (N-2-pyridinylcarbonyl-2-pyridinecarboximine)] were prepared by the Cu(II)-assisted hydrolysis of 2,4,6-tris(2-pyridyl)-1,3,5-triazine. Spectroscopic results indicate 5-coordinate, approx. square-pyramidal, geometry around the Cu(II) ion. Half-field absorption in the  $\Delta$ Ms =  $\pm 2$  region of the X-band ESR powder spectra was observed for the dimeric species.

L5 ANSWER 61 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1988:178938 CAPLUS  
 DN 108:178938  
 TI Preparation of new mono and polynuclear bis(triphenylphosphine) copper(I) derivatives containing mono and bidentate N-heterocycles, 8-hydroxyquinoline and oxalate ligands

AU Diez, Josefina; Falagan, Santiago; Gamasa, Pilar; Gimeno, Jose  
 CS Dep. Quim. Organomet., Univ. Oviedo, Oviedo, 33071, Spain  
 SO Polyhedron (1988), 7(1), 37-42  
 CODEN: PLYHDE; ISSN: 0277-5387  
 DT Journal  
 LA English  
 AB Cu(HL)(PPh<sub>3</sub>)<sub>2</sub> [H<sub>2</sub>L = bibenzimidazole, tetramethylbiimidazole], CuL(PPh<sub>3</sub>)<sub>2</sub> and Cu<sub>2</sub>(μ-C<sub>2</sub>O<sub>4</sub>)(PPh<sub>3</sub>)<sub>4</sub> (HL<sub>1</sub> = oxine) were obtained by reaction of Cu(acac)(PPh<sub>3</sub>)<sub>2</sub> (Hacac = acetylacetonate) with the corresponding ligands. The reaction of [Cu(CH<sub>3</sub>CN)<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>][BF<sub>4</sub>] with imidazole or pyrazole derivs. renders tetrahedral [Cu(L<sub>2</sub>)<sub>x</sub>(PPh<sub>3</sub>)<sub>2</sub>][BF<sub>4</sub>] [x = 1, L<sub>2</sub> = 2,2'-biimidazole, H<sub>2</sub>L; x = 2, L<sub>2</sub> = imidazole, pyrazole]; [Cu<sub>2</sub>(μ-L)(PPh<sub>3</sub>)<sub>2</sub>]<sub>2</sub> are formed when the corresponding bibenzimidazolate or tetramethylbiimidazolate are used as ligands. The structures of the resulting complexes were elucidated by IR spectroscopy, <sup>1</sup>H, <sup>31</sup>P{<sup>1</sup>H} NMR, mol. weight and conductance studies.

L5 ANSWER 62 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1988:105246 CAPLUS  
 DN 108:105246  
 TI Metal complexes of anxiolytic drugs. Crystal structure and electronic properties of dimeric oxalato complex of copper(II) bromazepam  
 AU Real, Jose A.; Borrás, Joaquín; Solans, Xavier; Font-Altaba, Manuel  
 CS Fac. Farm., Univ. Valencia, Valencia, Spain  
 SO Transition Metal Chemistry (Dordrecht, Netherlands) (1987), 12(3), 254-6  
 CODEN: TMCHDN; ISSN: 0340-4285  
 DT Journal  
 LA English  
 AB [Cu<sub>2</sub>L<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)](PF<sub>6</sub>)<sub>1.5</sub>(ClO<sub>4</sub>)<sub>0.5</sub>·1.5H<sub>2</sub>O (I; L = bromazepam) was prepared. Its crystal structure, solved at room temperature, consists of dimer units bridged by oxalate ligands. Each Cu ion is surrounded by 2 nitrogens of L and 2 oxygens of the oxalate ligand; a mol. of H<sub>2</sub>O occupies the apical site. The magnetic properties of I were studied at 30-300 K. The molar magnetic susceptibility closely follows the behavior expected for an antiferromagnetically coupled Cu(II) binuclear complex with a singlet-triplet energy gap, J = -349 cm<sup>-1</sup>.

L5 ANSWER 63 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1988:48120 CAPLUS  
 DN 108:48120  
 TI Extremely weak magnetic exchange interactions in terpy-containing copper(II) dimer. Crystal and molecular structure of Cu(terpy)(CA)·H<sub>2</sub>O and [Cu<sub>2</sub>(terpy)<sub>2</sub>(CA)](PF<sub>6</sub>)<sub>2</sub> complexes (terpy = 2,2':6',2''-terpyridine, CA = dianion of chloranilic acid)  
 AU Folgado, José V.; Ibanez, Rafael; Coronado, Eugenio; Beltrán, Daniel; Savariault, Jean M.; Galy, Jean  
 CS Dep. Quim. Inorg., Univ. Valencia, Valencia, Spain  
 SO Inorganic Chemistry (1988), 27(1), 19-26  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB Cu(terpy)(CA)·H<sub>2</sub>O (I; terpy = 2,2':6',2''-terpyridine; H<sub>2</sub>CA = chloroanilic acid) and [Cu<sub>2</sub>(terpy)<sub>2</sub>L]<sub>2</sub>X<sub>2</sub> (H<sub>2</sub>L = H<sub>2</sub>CA, H<sub>2</sub>C<sub>2</sub>O<sub>4</sub>; X = ClO<sub>4</sub>- or PF<sub>6</sub>-) were prepared. The x-ray crystal structures of I and [Cu<sub>2</sub>(terpy)<sub>2</sub>(CA)](PF<sub>6</sub>)<sub>2</sub> (II) are presented. [Cu<sub>2</sub>(terpy)<sub>2</sub>(CA)]<sub>2</sub> are isostructural. I is associated in pseudodimeric entities formed by 2 Cu(terpy)(CA)·H<sub>2</sub>O moieties connected via H bonding whereas the structure of II is built-up by the dimeric [Cu<sub>2</sub>(terpy)<sub>2</sub>(CA)]<sub>2</sub><sup>2+</sup> cations and PF<sub>6</sub>- anions. The Cu(II) ion coordination geometry is 5-coordinate and intermediate between trigonal bipyramidal and square pyramidal in I and close to square pyramidal in II. From variable-temperature magnetic susceptibility measurements (4.2-300 K) weak antiferromagnetic exchange interactions (2J = -1.6 cm<sup>-1</sup>) are seen for the [Cu<sub>2</sub>(terpy)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)](PF<sub>6</sub>)<sub>2</sub> whereas no exchange interactions are detected for the other complexes. Room-temperature ESR spectra of all 4 complexes show the ΔM<sub>s</sub> = ±2 forbidden transition. The observation of temperature-dependent singlet-to-triplet forbidden ESR transitions (at 100-500 K) in the CA complexes allows one to determine the exchange parameters (0.04-0.12 cm<sup>-1</sup>) as

well as the thermal evolution. The observed exchange interactions are discussed on the basis of the structural findings. In particular, a discussion about the feasible paths of exchange interactions in I is presented.

L5 ANSWER 64 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1987:167513 CAPLUS

DN 106:167513

TI Anisotropic exchange in dinuclear complexes with polyatomic bridges. Crystal and molecular structure and EPR spectra of ( $\mu$ -oxalato)bis(1,10-phenanthroline)dicopper(II) dinitrate

AU Bencini, Alessandro; Fabretti, Antonio C.; Zanchini, Claudia; Zannini, Paolo

CS ISSECC, CNR, Florence, Italy

SO Inorganic Chemistry (1987), 26(9), 1445-9

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB The title compound is triclinic, space group  $P_{21}2_12_1$ , with  $a$  9.977(6),  $b$  9.658(6),  $c$  7.036 (3) Å,  $\alpha$  108.03 (4),  $\beta$  95.40,  $\gamma$  90, 22 (4)°;  $Z$  = 2. The least-squares refinement of the structure led to a  $R$  = 0.036. At coordinates, bond lengths, and bond angles are given. Single-crystal EPR spectra were recorded at X-band frequency at 77 K. The zero-field splitting tensor is largely misaligned from the  $g$  tensor. Exchange contributions to the anisotropic spin-spin interaction are operative. The relative influences of the dipolar magnetic and the anisotropic exchange interactions in determining the zero-field splitting in oxalato-bridged Cu(II) dimers are discussed.

L5 ANSWER 65 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:617841 CAPLUS

DN 105:217841

TI Hexafluorophosphate and oxalate complexes of 4-methoxy-2-(5-methoxy-3-methylpyrazol-1-yl)-6-methylpyrimidine with cobalt(II), nickel(II) and copper(II)

AU Tormos, J. G.; Molla, M. C.; Garcia, J.

CS Fac. Farm., Univ. Valencia, Valencia, Spain

SO Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (

1986), 16(6), 821-9

CODEN: SRIMCN; ISSN: 0094-5714

DT Journal

LA English

AB  $ML_3(PF_6)_2$  ( $L$  = 4-methoxy-2-(5-methoxy-3-methylpyrazol-1-yl)-6-methylpyrimidine;  $M$  = Co, Cu, Ni),  $CuL_2(PF_6)_2$ ,  $CoL(C_2O_4)$ ,  $NiL(C_2O_4) \cdot H_2O$ ,  $[Cu_2L_2(C_2O_4)](ClO_4)_2$ , and  $[Cu_2L_2(C_2O_4)]NO_3 \cdot H_2O$  were prepared and characterized through elemental anal., conductivity measurements, electronic and IR spectra, and magnetic measurements.  $[ML_3](PF_6)_2$  and  $[CuL_2](PF_6)_2$  are monomeric. Oxalate acts as a bidentate bridge to form compds. with probable dimeric (Cu(II)) or polymeric (Co(II) and Ni(II)) structures.

L5 ANSWER 66 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:507056 CAPLUS

DN 105:107056

TI EPR evidence for an unexpected symmetric dinuclear species present in the lattice of an asymmetric dinuclear copper complex

AU Bencini, Alessandro; Gatteschi, Dante; Zanchini, Claudia; Kahn, Olivier; Verdager, Michel; Julve, Miguel

CS Dep. Chem., Univ. Florence, Florence, 50144, Italy

SO Inorganic Chemistry (1986), 25(18), 3181-3

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB The low-temperature single-crystal EPR spectra of  $[(dien)Cu(ox)Cu(tmen)(H_2O)_2](ClO_4)_2$  ( $dien$  = diethylenetriamine;  $ox$  = oxalato;  $tmen$  =  $N,N,N',N'$ -tetramethylethylenediamine) revealed that the paramagnetic species that causes the deviation of the magnetic susceptibility from the Bleaney-Bowers equation is a spin triplet containing 2 equivalent Cu ions. Comparison of the magnetic properties of the impurity with those reported in the literature for similar compds. indicates that

[(dien)Cu(ox)Cu(dien)]<sup>2+</sup> species are present in the lattice.

L5 ANSWER 67 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1985:16519 CAPLUS

DN 102:16519

TI Copper(II), a chemical Janus: two different (oxalato)(bipyridyl)copper(II) complexes in one single crystal. Structure and magnetic properties

AU Julve, Miguel; Faus, Juan; Verdaguer, Michel; Gleizes, Alain

CS Dep. Chim. Inorg., Fac. Cienc. Quim., Valencia, Spain

SO Journal of the American Chemical Society (1984), 106(26), 8306-8

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

AB [Cu<sub>2</sub>(bpy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)] [Cu(bpy)(C<sub>2</sub>O<sub>4</sub>)](NO<sub>3</sub>)<sub>2</sub> (bpy = 2,2'-bipyridine), prepared from [Cu(bpy)](NO<sub>3</sub>)<sub>2</sub> and aqueous Li<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, crystallizes in the monoclinic system, space group C<sub>2</sub>/c, with a 21.739(2), b 10.458(1), c 16.023(2) Å, β 95.69(1)°, and R = 0.029, R<sub>w</sub> = 0.051 for 3290 reflections with I > 3σ(I). Cu in Cu(bpy)(C<sub>2</sub>O<sub>4</sub>) is nearly square planar with bidentate coordination of bpy and C<sub>2</sub>O<sub>4</sub><sup>2-</sup>. Cu in [Cu<sub>2</sub>(bpy)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)]<sup>2+</sup> is square pyramidal with apical H<sub>2</sub>O; the oxalate is tetradentate bridging. The thermal variation of magnetic susceptibility shows strong antiferromagnetic interaction within the binuclear unit and no interaction between the 2 Cu species at 20-300K.

L5 ANSWER 68 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:603203 CAPLUS

DN 101:203203

TI Design of μ-oxalato copper(II) binuclear complexes exhibiting expected magnetic properties

AU Julve, Miguel; Verdaguer, Michel; Gleizes, Alain; Philoche-Levisalles, Michele; Kahn, Olivier

CS Lab. Spectrochim. Elem. Transition, Univ. Paris-Sud, Orsay, 91405, Fr.

SO Inorganic Chemistry (1984), 23(23), 3808-18

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Some basic concepts from the theory of the interaction between magnetic metal centers in coupled polymetallic systems were used to design μ-oxalato Cu(II) binuclear complexes in which the magnitude of the antiferromagnetic coupling can be tuned. The 2 main concepts are those of magnetic orbital, defined as the singly occupied MO in a monomeric fragment, and of overlap between 2 magnetic orbitals in the binuclear unit. The magnitude of the antiferromagnetic interaction is expected to vary as the square of this overlap. In a [LCu(C<sub>2</sub>O<sub>4</sub>)CuL<sub>1</sub>]<sup>2+</sup> binuclear cation, where L and L<sub>1</sub> are terminal ligands, the 2 monomeric fragments LCu(C<sub>2</sub>O<sub>4</sub>) and L<sub>1</sub>Cu(C<sub>2</sub>O<sub>4</sub>) do actually exist. According to the nature of L and L<sub>1</sub>, the spatial orientation of the magnetic orbitals may be predicted, as well as the overlap between them. To test this approach, the preparation, crystal structures, and magnetic properties of 3 new complexes are described: [tmen(H<sub>2</sub>O)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(H<sub>2</sub>O)tmen](ClO<sub>4</sub>)<sub>2</sub>·1.25H<sub>2</sub>O (I), [dienCu(C<sub>2</sub>O<sub>4</sub>)Cu(H<sub>2</sub>O)<sub>2</sub>tmen](ClO<sub>4</sub>)<sub>2</sub> (II), and [tmen(2-MeIm)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(2-MeIm)tmen](PF<sub>6</sub>)<sub>2</sub> (III), (tmen = Me<sub>2</sub>NC<sub>2</sub>H<sub>4</sub>NMe<sub>2</sub>, dien = diethylenetriamine, 2-MeIm = 2-methylimidazole). Lattice and mol. parameters are reported. Each Cu atom in I is in a square-pyramidal environment with the 2 N atoms of tmen and 2 O atoms of C<sub>2</sub>O<sub>4</sub><sup>2-</sup> in the basal plane and a water mol. occupying the apical position. In II, on the dien side, the 4 nearest neighbors of Cu are the 3 N atoms of dien and only 1 O atom of C<sub>2</sub>O<sub>4</sub><sup>2-</sup>; on the tmen side, the basal plane is again made of 2 O atoms of C<sub>2</sub>O<sub>4</sub><sup>2-</sup> and 2 N atoms of tmen. The environment of each Cu in III is intermediate between the square pyramid with only 1 O atom of C<sub>2</sub>O<sub>4</sub><sup>2-</sup> in the basal plane and the trigonal bipyramid. The magnetic properties of the 3 compds. were studied at 2-300 K and the singlet-triplet energy gaps deduced from the magnetic data are -385.4 cm<sup>-1</sup> for I, -75.5 cm<sup>-1</sup> for II, and -13.8 cm<sup>-1</sup> for III. These values are compared to the previsions and the perspectives and limits of such a mol. engineering of the coupled systems are discussed.

L5 ANSWER 69 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:598387 CAPLUS

DN 101:198387

TI Ab initio direct calculation of the singlet-triplet splitting in a  
 $\mu$ -oxalato copper(II) binuclear complex  
 AU Charlot, M. F.; Verdaguer, M.; Journaux, Y.; De Loth, P.; Daudey, J. P.  
 CS Lab. Spectrochim. Elem. Transition, Univ. Paris Sud, Orsay, 91405, Fr.  
 SO Inorganic Chemistry (1984), 23(23), 3802-8  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB The singlet-triplet (S-T) splitting was calculated of  $\mu$ -oxalato  
 bis((N,N,N',N'-tetramethyl-1,2-ethanediamine)copper(II)) perchlorate in  
 an ab initio scheme. The method, based on a perturbation development of  
 the CI problem, directly gives the S-T energy separation, after an ab initio  
 SCF-MO calcn. on the open-shell system, using pseudopotentials. The 2K<sub>B</sub>  
 ferromagnetic potential-exchange contribution is important (720 cm<sup>-1</sup>) and  
 not balanced by the 2nd-order kinetic-exchange mechanism (.apprx.-450  
 cm<sup>-1</sup>). The other 2nd-order contributions are the double-spin polarization  
 (-38 cm<sup>-1</sup>), the ligand-metal charge transfer (-146 cm<sup>-1</sup>), and the  
 kinetic-exchange + polarization (-177 cm<sup>-1</sup>). The 4th-order terms allow  
 one to reach a total value of -295 cm<sup>-1</sup> not too far from the exptl. one  
 -385 cm<sup>-1</sup>. The magnitude of the different contributions is discussed and  
 compared to that of a  $\mu$ -dithiooxamido copper(II) binuclear complex.

L5 ANSWER 70 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1984:542795 CAPLUS  
 DN 101:142795  
 TI Exchange coupling in dinuclear copper(II) complexes with oxalato,  
 oxamidato and oxamato ligands  
 AU Bencini, A.; Benelli, C.; Gatteschi, D.; Zanchini, C.; Fabretti, A. C.;  
 Franchini, G. C.  
 CS Dep. Chem., Univ. Florence, Florence, Italy  
 SO Inorganica Chimica Acta (1984), 86(3), 169-72  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 AB [Cu<sub>2</sub>(phen)<sub>2</sub>L](NO<sub>3</sub>)<sub>2</sub>.nH<sub>2</sub>O (I) (H<sub>2</sub>L = oxamide, oxamic acid, oxalic acid, n =  
 1.5, 3, 0, phen = 1,10-phenanthroline) were prepared. The effect of the  
 ligands on the extent of the antiferromagnetic coupling between the 2  
 metal ions was studied in I, [Cu<sub>2</sub>(dpa)<sub>2</sub>L<sub>1</sub>](NO<sub>3</sub>)<sub>2</sub> (dpa =  
 2,2'-dipyridylamine, H<sub>2</sub>L<sub>1</sub> = oxamide), and [Cu<sub>2</sub>L<sub>2</sub>](BPh<sub>4</sub>)<sub>2</sub>.Me<sub>2</sub>CO (H<sub>2</sub>L<sub>2</sub> =  
 bis(6-ethyl-3,6-diazaoctyl)oxamide). Magnetic susceptibility measurements  
 showed that the single-triplet splitting are 330-550 cm<sup>-1</sup>; J increases in  
 the order oxalato < oxamato < oxamidato.

L5 ANSWER 71 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1984:113946 CAPLUS  
 DN 100:113946  
 TI Interactions in copper(II)-copper(II), vanadyl(II)-vanadyl(II), and  
 copper(II)-vanadyl(II) pairs through oxalato bridging ligand  
 AU Julve, Miguel; Verdaguer, Michel; Charlot, Marie France; Kahn, Olivier;  
 Claude, Renee  
 CS Lab. Spectrochim. Elem. Transition, Univ. Paris-Sud, Orsay, 91405, Fr.  
 SO Inorganica Chimica Acta (1984), 82(1), 5-12  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 AB To compare the interaction in Cu(II)Cu(II), VO(II)VO(II), and Cu(II)VO(II)  
 pairs through the same oxalato bridging ligand,  
 (acac)VO(C<sub>2</sub>O<sub>4</sub>)VO(acac).4H<sub>2</sub>O (I) and (tmen)Cu(C<sub>2</sub>O<sub>4</sub>)VO(C<sub>2</sub>O<sub>4</sub>).3H<sub>2</sub>O (II)  
 (Hacac = acetylacetone and tmen = N,N,N',N'-tetramethylethylenediamine)  
 were prepared and compared with [tmen(H<sub>2</sub>O)Cu(C<sub>2</sub>O<sub>4</sub>)Cu(H<sub>2</sub>O)tmen](ClO<sub>4</sub>)<sub>2</sub>.1.25H<sub>2</sub>O  
 (III). The singlet-triplet energy gaps arising from the intramol.  
 interaction, determined from the magnetic data, are -385.4 cm<sup>-1</sup> in III, -5.75  
 cm<sup>-1</sup> in I and |J| < 1 cm<sup>-1</sup> in II. The EPR spectrum of II shows a  
 transition in a triplet state with a singlet-triplet energy gap larger, in  
 absolute value, than the incident quantum (.apprx.0.3 cm<sup>-1</sup> in X-band). To  
 obtain this result, the spectrum was compared to those of the monomeric  
 species (tmen)Cu(C<sub>2</sub>O<sub>4</sub>).4H<sub>2</sub>O and (NH<sub>4</sub>)<sub>2</sub>VO(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>.2H<sub>2</sub>O. The magnitude of  
 the singlet-triplet gaps J was rationalized within the framework of an  
 orbital model. II is a new heterobimetallic compound in which the

interaction is expected to be purely ferromagnetic owing to the strict orthogonality of the magnetic orbitals. Finally, an explanation of the absence of zero field splitting in the triplet state of III is proposed. The anisotropic exchange interaction in III might be considered as being proportional to the isotropic exchange interaction in II.

L5 ANSWER 72 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:43390 CAPLUS

DN 100:43390

TI The structures of two oxalato-bridged copper dimers;  
[Cu<sub>2</sub>(Me<sub>4</sub>en)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub>·2H<sub>2</sub>O and [Cu<sub>2</sub>(Et<sub>5</sub>dien)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)](PF<sub>6</sub>)<sub>2</sub>

AU Sletten, Jorunn

CS Dep. Chem., Univ. Bergen, Bergen, N-5000, Norway

SO Acta Chemica Scandinavica, Series A: Physical and Inorganic Chemistry (1983), A37(7), 569-78

CODEN: ACAPCT; ISSN: 0302-4377

DT Journal

LA English

AB The structures of [Cu<sub>2</sub>(Me<sub>4</sub>en)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)(H<sub>3</sub>O)<sub>2</sub>](PF<sub>6</sub>)<sub>2</sub>·2H<sub>2</sub>O and [Cu<sub>2</sub>(Et<sub>5</sub>dien)<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)](PF<sub>6</sub>)<sub>2</sub>, where Me<sub>4</sub>en is N, N, N', N'', N'''-pentaethyldiehylenetriamine, were determined by using heavy-atom x-ray methods. The Me<sub>4</sub>en-compound is triclinic, space group P<sub>2</sub><sub>1</sub>h<sub>1</sub>1<sub>2</sub>, with a 7.932(5), b 8.117(7), c 12.089(15) Å, α 96.89(9), β 97.03(8), and γ 102.44(6)°; A = 1. The structure was refined to an R of 0.053 using 1353 reflections. The Et<sub>5</sub>dien compound is monoclinic, space Group I2/c, with a 13.436(9) b 22.29(2), c 14.59(1) Å, and β 103.68(7)°; Z = 4, and was refined to an R of 0.045 using 2112 reflections. Both compds. are centrosym. binuclear complexes bridged by an oxalate group. The Cu coordination in the Me<sub>4</sub>en compound is slightly distorted square pyramidal with the bridging group occupying 2 equatorial coordination sites and a H<sub>2</sub>O mol. in the apex position; in the Et<sub>5</sub>dien compound a geometry intermediate between square pyramidal and trigonal bipyramidal is found; the oxalate O atoms occupies 1 equatorial and 1 axial position. Atomic coordinates are given.

L5 ANSWER 73 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:624129 CAPLUS

DN 99:224129

TI Monomeric and dimeric copper(II) complexes composed of some terdentate Schiff bases and oxalate, oxamate, azide, thiocyanate or cyanate ions

AU Nakao, Yasuo; Yamazaki, Mitsuhiro; Suzuki, Shinnichiro; Mori, Wasuke; Nakahara, Akitsugu; Matsumoto, Keiji; Ooi, Shun'ichiro

CS Fac. Educ., Okayama Univ., Okayama, 700, Japan

SO Inorganica Chimica Acta (1983), 74, 159-67

CODEN: ICHAA3; ISSN: 0020-1693

DT Journal

LA English

AB Monomeric and dimeric Cu(II) complexes containing the Schiff bases (L, L<sub>1</sub>, HL<sub>2</sub>) derived from 2-pyridinecarbaldehyde and histamine, 2-(2-aminoethyl)pyridine, or β-alanine, resp., and oxalate (ox) oxamate (om), N<sub>3</sub><sup>-</sup>, SCN<sup>-</sup>, or OCN<sup>-</sup> were prepared and characterized from electronic, IR and ESR spectra, and magnetic susceptibilities. The crystals of monomeric [CuL(N<sub>3</sub>)<sub>2</sub>] are triclinic, with a 10.262(8), b 9.177(6), c 7.688(5) Å, α 104.42(4), β 94.09(4), γ 92.64(4)°, Z = 2, and space group P<sub>2</sub><sub>1</sub>h<sub>1</sub>1<sub>2</sub>. The 5-coordinate geometry around Cu is intermediate between trigonal-bipyramid and square-pyramid. The half-field absorption in the Δ<sub>M</sub>s = 2 region of powdered X-band ESR spectra was scarcely observed for [CuL<sub>1</sub>(N<sub>3</sub>)<sub>2</sub>], [CuL<sub>1</sub>(NCS)<sub>2</sub>], [CuL<sub>1</sub>(NCO)<sub>2</sub>] and [CuL(N<sub>3</sub>)<sub>2</sub>]. Dimeric [Cu<sub>2</sub>L<sub>2</sub>(N<sub>3</sub>)<sub>3</sub>]Cl·2H<sub>2</sub>O and [Cu<sub>2</sub>L<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub> exhibited the half-field absorption in the same region. However, an exchange interaction was hardly observed down to 4.2 K in the magnetic susceptibility measurement for [Cu<sub>2</sub>L<sub>2</sub>(N<sub>3</sub>)<sub>3</sub>]Cl·2H<sub>2</sub>O. The susceptibility of an oxalate-bridged [Cu<sub>2</sub>L<sub>2</sub>(ox)](ClO<sub>4</sub>)<sub>2</sub>, showed an antiferromagnetic interaction (J = -21.5 cm<sup>-1</sup>) and the X-band ESR spectrum for the powdered sample showed a very weak absorption for the triplet state of such a dimer in the Δ<sub>M</sub>s = 2 region.

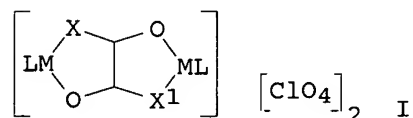
L5 ANSWER 74 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:45867 CAPLUS



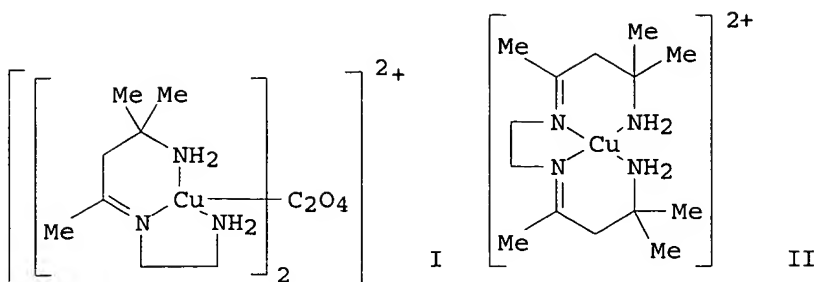
DN 98:45867  
 TI Tunable exchange interaction in  $\mu$ -oxalato copper(II) dinuclear complexes  
 AU Julve, Miguel; Verdaguer, Michel; Kahn, Olivier; Gleizes, Alain; Philoche-Levisalles, Michele  
 CS Lab. Spectrochim. Elements Transit., Univ. Paris Sud, Orsay, 91405, Fr.  
 SO Inorganic Chemistry (1983), 22(2), 368-70  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal  
 LA English  
 AB A method of synthesis leading to eventually asym. dinuclear cations  $[\text{LCu}(\text{C}_2\text{O}_4)\text{CuL}']_2^{2+}$  is described. In  $[\text{tmen}(\text{H}_2\text{O})\text{Cu}(\text{C}_2\text{O}_4)\text{Cu}(\text{H}_2\text{O})\text{tmen}](\text{ClO}_4)_2 \cdot 1.25\text{H}_2\text{O}$  (tmen = 1,1,4,4-tetramethylethylenediamine) the coordination of each Cu(II) is 4 + 1 with the N atoms of tmen and 2 O atoms of the oxalato ligand as nearest neighbors and a H<sub>2</sub>O mol. in apical position. The relative orientations of the magnetic orbitals are particularly favorable to give rise to a strong antiferromagnetic coupling and J is -385.4 cm<sup>-1</sup>. In  $[\text{dienCu}(\text{C}_2\text{O}_4)\text{Cu}(\text{H}_2\text{O})_2\text{tmen}](\text{ClO}_4)_2$  (I) (dien = diethylenetriamine) the coordination of each Cu(II) is 4 + 2. On the tmen side, the 4 nearest neighbors are again the N atoms of tmen and 2 O atoms of C<sub>2</sub>O<sub>4</sub>, with 2 H<sub>2</sub>O mols. in apical position. On the dien side, the 4 nearest neighbors are the N atoms of dien and 1 O atom of C<sub>2</sub>O<sub>4</sub>, with in apical position a second atom of C<sub>2</sub>O<sub>4</sub> and an O atom belonging to the oxalate bridge to another dinuclear unit. In I, the 2 magnetic orbitals overlap only on 1 side of the Cu(C<sub>2</sub>O<sub>4</sub>)Cu network and J is -75.5 cm<sup>-1</sup>.

L5 ANSWER 75 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1982:227891 CAPLUS  
 DN 96:227891  
 TI Five coordinate binuclear nickel(II) and copper(II) complexes of 1,5,9-triazacyclotridecane with  $\mu$ -oxamido,  $\mu$ -oxamato, and  $\mu$ -oxalato bridges  
 AU Nonoyama, Matsuo; Nonoyama, Kiyoko  
 CS Dep. Chem., Nagoya Univ., Nagoya, 464, Japan  
 SO Journal of Inorganic and Nuclear Chemistry (1981), 43(10), 2567-70  
 CODEN: JINCAO; ISSN: 0022-1902  
 DT Journal  
 LA English  
 GI



AB The oxamido-, oxalato-, and oxamato-bridged 5-coordinate binuclear complexes I (X, X1 = NH, NH; O, O; NH, O, resp.; M = Ni, Cu; L = 1,5,9-triazacyclotridecane) were prepared and characterized by elemental anal., magnetism, conductivity, IR, and electronic spectra. L coordinates through its 3 N atoms. In the proposed square-pyramidal structures, the bridging ligand donor atoms occupy equatorial sites for both metal atoms.

L5 ANSWER 76 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1981:24190 CAPLUS  
 DN 94:24190  
 TI Some metal-ion complexes with ligands formed by reactions of amines with aliphatic carbonyl compounds. VII. Copper(II) compounds of some  $\beta$ -imino amines formed by reaction of copper(II) chelate amine complexes with 4-amino-4-methylpentan-2-one  
 AU Morgan, Keith R.; Martin, John W. L.; Curtis, Neil F.  
 CS Chem. Dep., Victoria Univ., Wellington, N. Z.  
 SO Australian Journal of Chemistry (1979), 32(11), 2371-80  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DT Journal  
 LA English



AB Compds. of Cu(II) with chelated  $\beta$ -imino amines are formed by reactions between 4-amino-4-methylpentan-2-one (amp) and Cu(II) complexes of ethane-1,2-diamine, propane-1,2- and -1,3-diamine, meso-1,2-diphenylethane-1,2-diamine, 2-(2-aminoethyl)pyridine, 3-azapentane-1,5-diamine, 3-azaheptane-1,6-diamine, 4-azaheptane-1,7-diamine, 3,6-diazaoctane-1,8-diamine, 4,8-diazaundecane-1,11-diamine, 3-(2-aminoethyl)-3-azapentane-1,5-diamine and 4,6,6-trimethyl-3,7-diazanon-3-ene-1,9-diamine. Compds. with one  $\beta$ -imino amine group, e.g. I, were formed for all the amines, except 1,2-diphenylethane-1,2-diamine and propane-1,3-diamine, and compds. with tetradentate ligands with two  $\beta$ -imino amine groups, e.g. II, were formed with the aliphatic diamines. The imine group of the compds. is relatively resistant to hydrolysis.

L5 ANSWER 77 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1980:596839 CAPLUS

DN 93:196839

TI Synthesis of binuclear copper(II) complexes with  $\mu$ -oxamido,  $\mu$ -oxamato, and  $\mu$ -oxalato-bridges

AU Nonoyama, Kiyoko; Ojima, Heijiro; Ohki, Kosuke; Nonoyama, Matsuo

CS Hayashi Junior Coll., Aichi, 483, Japan

SO Inorganica Chimica Acta (1980), 41(2), 155-9

CODEN: ICHAA3; ISSN: 0020-1693

DT Journal

LA English

AB  $\mu$ -Oxamido-,  $\mu$ -oxamato-, and  $\mu$ -oxalato-bridged binuclear Cu(II) complexes  $[\text{Cu}_2(\text{bridge})\text{L}_2]^{2+}$  coordinated with another ligand (L) such as 2,2'-bipyridine, 2,2'-dipyridylamine, N,N,N',N''-tetramethylethylenediamine, 2-(2-aminoethyl)pyridine, N,N,N',N'',N'''-pentamethyldiethylenetriamine, N,N,N',N'',N'''-tetraethyldiethylenetriamine, and N,N,N',N'',N'''-pentaethyldiethylenetriamine were prepared and characterized by IR and electronic spectra and magnetic moments at room temperature. The complexes are square-planar or tetragonal octahedral for the bidentate L ligands, while they are 5-coordinate for the terdentate L ligands. The magnetic moments of these complexes depend upon the bridges as well as the L ligands. The moments of the complexes with bidentate L are all subnormal and decrease in the order:  $\mu$ -oxalato- >  $\mu$ -oxamato- >  $\mu$ -oxamido-bridge. The moments of the complexes with terdentate L are normal for a  $\mu$ -oxalato-bridge but subnormal for a  $\mu$ -oxamido-bridge. Magnetic Cu-Cu interaction seems to be more effective through a  $\mu$ -oxamido-bridge than through  $\mu$ -oxamato- and  $\mu$ -oxalato-bridges.

L5 ANSWER 78 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1980:560440 CAPLUS

DN 93:160440

TI Compounds of cobalt(II), nickel(II) and copper(II) with 2,4,4,9-tetramethyl-1,5,9-triazacyclododec-1-ene

AU Martin, John W. L.; Curtis, Neil F.

CS Chem. Dep., Victoria Univ. Wellington, Wellington, N. Z.

SO Australian Journal of Chemistry (1980), 33(6), 1241-9

CODEN: AJCHAS; ISSN: 0004-9425

DT Journal

LA English

AB Compds. of the macrocycle 2,4,4,9-tetramethyl-1,5,9-triazacyclododec-1-ene

(dla) with Co, Ni, and Cu are formed by reaction of Me<sub>2</sub>CO with 4-methyl-4-azaheptane-1,7-diamine complexes with these metals. The preps. of M(dla)(NCS)<sub>2</sub> (M = Co, Ni, Cu), [M'(dla)(en)](ClO<sub>4</sub>)<sub>2</sub>, [{M'(dla)(OH)}<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>, [{M'(dla)}<sub>2</sub>CO<sub>3</sub>](ClO<sub>4</sub>)<sub>2</sub>, [M'(dla)(acac)]ClO<sub>4</sub> (Hacac = acetylacetone), [{M'(dla)}<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> (M' = Ni, Cu), and [{Ni(dla)Cl}<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub> are reported. The compds. are all assigned 5-coordinate structures. The compds. [{M'(dla)}<sub>2</sub>CO<sub>3</sub>](ClO<sub>4</sub>)<sub>2</sub>, [{Cu(dla)(OH)}<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>, and {Cu(dla)}<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> show appreciable antiferromagnetic spin-coupling.

L5 ANSWER 79 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1980:173683 CAPLUS

DN 92:173683

TI Synthesis and characterization of copper(II) squarate complexes

AU Reinprecht, James T.; Miller, James G.; Vogel, Glenn C.; Haddad, Muin S.; Hendrickson, David N.

CS Dep. Chem., Ithaca Coll., Ithaca, NY, 14850, USA

SO Inorganic Chemistry (1980), 19(4), 927-31

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB A number of new Cu(II) complexes containing an oxocarbon dianion (squarate, croconate or rhodizonate ion) and nitrogenous counterligands were prepared. Both monomeric and dimeric mixed-ligand complexes were isolated when the oxocarbon dianion used was the squarate ion. In these dimeric complexes the squarate ion functions as a bis-monodentate bridging ligand when the counterligand is 2,2'-bipyridine or 1,10-phenanthroline and is a bis-bidentate bridging ligand when the counterligand is 1,1,7,7-tetraethyldiethylenetriamine. In addition to normal spectral characterization, a temperature-dependent study of the magnetic susceptibility of several of the squarate dimers, indicating weak antiferromagnetic exchange interaction, is reported.

L5 ANSWER 80 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1978:415910 CAPLUS

DN 89:15910

TI Complexes of 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene with cobalt(II), nickel(II), and copper(II); x-ray structure determination of diisothiocyanato(2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene)nickel(II)

AU Martin, John W. L.; Johnston, James H.; Curtis, Neil F.

CS Chem. Dep., Victoria Univ., Wellington, N. Z.

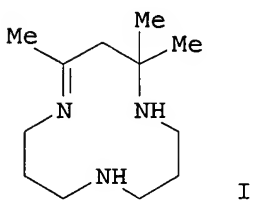
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1978), (1), 68-76

CODEN: JCDBTI; ISSN: 0300-9246

DT Journal

LA English

GI



AB Reactions of bis(4-azaheptane-1,7-diamine)metal(II) complexes (metal = M = Ni, Co, Cu) as their thiocyanate and perchlorate salts with Me<sub>2</sub>CO gave ML(NCS)<sub>2</sub> [L = 2,4,4-trimethyl-1,5,9-triazacyclododec-1-ene (I)] and [(ML)<sub>2</sub>(OH)<sub>2</sub>](ClO<sub>4</sub>)<sub>2</sub>, resp. With Ni(II), and to a lesser extent Cu(II), the di-μ-hydroxo dimer reacts with chelating anionic ligands to give [MLL<sub>1</sub>]X [L<sub>1</sub> = pentane-2,4-dionato (L<sub>2</sub>), acetato, μ-oxalato, 2-acetylphenolato; X = uncoordinated ClO<sub>4</sub>, NCS]. The complexes are 5-coordinate, except for [NiL(NCS)]<sub>2</sub>[C<sub>2</sub>O<sub>4</sub>] and NiLL<sub>2</sub>(NCS). The structure of NiL(NCS)<sub>2</sub> was determined by x-ray diffraction, and shows a distorted square-pyramidal arrangement about the Ni ion with a Me group in the

vacant octahedral site. The complexes were characterized by elemental anal., d-d and IR spectra, and room-temperature magnetic susceptibilities.  $[(\text{NiL})_2(\text{OH})_2][\text{ClO}_4]_2$  and  $[\text{CuLL}_2][\text{ClO}_4]$  obey the Curie-Weiss law at 100-300 K, whereas  $[(\text{CuL})_2(\text{OH})_2][\text{ClO}_4]_2$  shows appreciable antiferromagnetic spin coupling over this temperature range ( $2J = -120 \text{ cm}^{-1}$ ).

L5 ANSWER 81 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1977:163814 CAPLUS

DN 86:163814

TI Magnetic exchange interactions in transition metal dimers. 10.

Structural and magnetic characterization of oxalate-bridged, bis(1,1,4,7,7-pentaethyldiethylene triamine)oxalatodicopper tetraphenylborate and related dimers. Effects of nonbridging ligands and counterions on exchange interactions

AU Felthouse, Timothy R.; Laskowski, Edward J.; Hendrickson, David N.

CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA

SO Inorganic Chemistry (1977), 16(5), 1077-89

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB The structure of  $[\text{Cu}_2(\text{Et}_5\text{dien})_2(\text{C}_2\text{O}_4)](\text{BPh}_4)_2$ , where  $\text{Et}_5\text{dien}$  is 1,1,4,7,7-pentaethyldiethylenetriamine, was determined by heavy-atom least-square x-ray methods and refined to  $R_F$  0.069 and  $R_wF$  0.056 for 2979 reflections. The crystals are monoclinic, space group  $P2_1/n$ , with  $a$  9.776(5),  $b$  25.004(12),  $c$  14.551(6) Å, and  $\beta$  91.83(2)°;  $d(\text{exptl.}) = 1.25(2)$  and  $d(\text{calculated}) = 1.26$  for  $Z = 2$ . The compound is a  $\text{BPh}_4^-$  salt of an oxalate-bridged, centrosymmetric  $\text{Cu}(\text{II})$  dimeric cation. The oxalate dianion bridges in a bis-bidentate fashion between 2 distorted trigonal-bipyramidal (TBP) copper complexes with the oxalate dianion taking both an equatorial ( $\text{Cu}-\text{O}$  2.174(4) Å) and an axial ( $\text{Cu}-\text{O}$  1.972(4) Å) coordination site at each  $\text{Cu}(\text{II})$  ion. The  $\text{Cu}-\text{Cu}$  distance of 5.410(1) Å and the  $\text{Cu}-(\text{C}_2\text{O}_4)-\text{Cu}$  unit is planar. Variable-temperature (4.2-270 K) magnetic susceptibility data for this compound show a relatively large antiferromagnetic exchange interaction with a  $J$  value of  $-37.4 \text{ cm}^{-1}$ . Magnetic susceptibility data (4.2-270 K) and EPR spectra (X and Q band) are presented for the series of  $\mu$ -oxalato compds.  $[\text{Cu}_2(\text{"dien"})_2(\text{C}_2\text{O}_4)](\text{X})_2$ , where "dien" is variously  $\text{Et}_5\text{dien}$ ,  $\text{Me}_5\text{dien}$ ,  $\text{dpt}$  (dipropylenetriamine), and  $\text{dien}$  (diethylenetriamine) and  $\text{X}^-$  is either  $\text{BPh}_4^-$ ,  $\text{PF}_6^-$ , or  $\text{ClO}_4^-$ . The  $\text{Et}_5\text{dien}$  compounds have TBP  $\text{Cu}(\text{II})$  coordination geometries with the largest antiferromagnetic interactions. Replacing  $\text{Et}_5\text{dien}$  by any of the other 3 "dien" ligands distorts the  $\text{Cu}(\text{II})$  coordination geometry towards square pyramidal and decreases the antiferromagnetic interaction. A simplified MO anal. is presented to explain the changes in exchange interactions. The effects of nonbridging "dien" ligand and counterion are explained via the MO anal. And finally, magnetic susceptibility and EPR data are reported for some analogous squarate ( $\text{C}_4\text{O}_4^{2-}$ ), succinate ( $-\text{O}_2\text{CH}_2\text{CH}_2\text{O}_2^-$ ), and cyanate ( $\text{NCO}^-$ )-bridged  $\text{Cu}(\text{II})$  dimers.

L5 ANSWER 82 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1977:64551 CAPLUS

DN 86:64551

TI Structural and magnetic properties of copper(II) dimers bridged by

oxalate, azide, and cyanide ions; x-ray structures of

$[\text{Cu}_2\{\text{EtN}(\text{CH}_2\text{CH}_2\text{NEt}_2)_2\}_2(\text{C}_2\text{O}_4)][\text{BPh}_4]_2$  and  $[\text{Cu}_2\{\text{MeN}(\text{CH}_2\text{CH}_2\text{NMe}_2)_2\}_2(\text{N}_3)_2][\text{BPh}_4]_2$ . Role of transition-metal ion ground state in magnetic exchange interactions

AU Felthouse, Timothy R.; Laskowski, Edward J.; Bieksza, David S.; Hendrickson, David N.

CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA

SO Journal of the Chemical Society, Chemical Communications (1976), (19), 777-8

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

AB Variable-temperature magnetic susceptibility, ESR and single-crystal x-ray crystallog. data were determined to show that a predominantly  $d_{z^2}$   $\text{Cu}(\text{II})$  ground state can lead to appreciable magnetic exchange interactions through the extended bridges in  $[\text{Cu}_2\text{L}_2(\text{C}_2\text{O}_4)][\text{BPh}_4]_2$ ,  $[\text{Cu}_2(\text{L}_1)_2(\text{N}_3)_2][\text{BPh}_4]_2$ , and

[Cu<sub>2</sub>(L<sub>2</sub>)<sub>2</sub>(CN)] [PF<sub>6</sub>]<sub>3</sub> [L = EtN[(CH<sub>2</sub>)<sub>2</sub>NEt<sub>2</sub>]<sub>2</sub>, L<sub>1</sub> = MeN[(CH<sub>2</sub>)<sub>2</sub>NMe<sub>2</sub>]<sub>2</sub>, L<sub>2</sub> = N[(CH<sub>2</sub>)<sub>2</sub>NH<sub>2</sub>]<sub>3</sub>].

L5 ANSWER 83 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:488060 CAPLUS

DN 83:88060

TI Magnetic exchange interactions in transition metal dimers. V. Copper(II)-diethylenetriamine complexes with oxalate, cyanate, thiocyanate, and azide inner- and outer-sphere bridging units. Electron paramagnetic resonance of alkali halide pelleted copper complexes

AU Hall, Gretchen R.; Duggan, D. Michael; Hendrickson, David N.

CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA

SO Inorganic Chemistry (1975), 14(8), 1956-64

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. The magnetic susceptibility and EPR spectra of [Cu<sub>2</sub>(dien)<sub>2</sub>X<sub>2</sub>](BPh<sub>4</sub>)<sub>2</sub> (I) (dien = diethylenetriamine; X<sub>2</sub> = oxalate; X = N<sub>3</sub>, NCO, NCS) in alkali halide pellet form showed an antiferromagnetic interaction at 4.2°K. For I, X<sub>2</sub> = oxalate, this interaction was characterized by J = -7.4 cm<sup>-1</sup>, g = 2.16, θ = 1.3°. When the BPh<sub>4</sub> groups were replaced by ClO<sub>4</sub>, no exchange interaction was observed. The influences of structure, inner-sphere and outer-sphere bonding, and hydration are discussed.

L5 ANSWER 84 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:163555 CAPLUS

DN 82:163555

TI Structure of copper(II) thiosemicarbazidediacetate and copper(II) o-aminobenzaldehyde thiosemicarbazone oxalato complex

AU Rotaru, V. K.; Kiosse, G. A.; Malinovskii, T. I.; Gerbeleu, N. V.;

Shopron, M. V.; Bodyu, V. G.; Ablov, A. V.

CS Inst. Khim., Kishinev, USSR

SO Fiz. Mat. Metody Koord. Khim., Tezisy Dokl., Vses. Soveshch., 5th (1974), Meeting Date 1974, 137 Publisher: "Shtiintsa", Kishinev, USSR.

CODEN: 29UWAN

DT Conference

LA Russian

AB The structure of Cu thiosemicarbazidediacetate, Cu[(O<sub>2</sub>CCH<sub>2</sub>)<sub>2</sub>NNHC(S)NH<sub>2</sub>] is monoclinic, space group P2<sub>1</sub>/n, with a 14.04, b 14.46, c 9.47 Å, γ 105.5°, and Z = 8. Cu coordination is 5, intermediate between a square pyramid and a trigonal bipyramid. Carboxylic group bridges link the complexes in chains parallel to the z axis. The structure of [(CuL)(C<sub>2</sub>O<sub>4</sub>(CuL))<sub>2</sub> + [Cu(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>]<sub>2</sub> · H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> · 6H<sub>2</sub>O, where L = H<sub>2</sub>NC(S)NHNCH(C<sub>6</sub>H<sub>4</sub>)NH<sub>2</sub>, is triclinic, space group P<sub>1</sub>h<sub>1</sub>vin.1, with a 9.75, b 9.80, c 11.90 Å, α 81.20°, β 92°, and γ 122°. In the cation, the nearly planar ligand L is tridentate and the (C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>- is a bridging group. The H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> mol. is between the columns of complexes parallel to z axis.

L5 ANSWER 85 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1974:457719 CAPLUS

DN 81:57719

TI Preparation of γ-diamminecopper(II) and the study of its structure

AU Langfelderova, H.; Garaj, J.; Gazo, J.

CS Slovak Tech. Univ., Bratislava, Czech.

SO Chemicke Zvesti (1974), 28(2), 173-9

CODEN: CHZVAN; ISSN: 0366-6352

DT Journal

LA German

AB The formation of γ-Cu(C<sub>2</sub>O<sub>4</sub>)(NH<sub>3</sub>)<sub>2</sub> by the thermal decomposition of [Cu(NH<sub>3</sub>)<sub>5</sub>](C<sub>2</sub>O<sub>4</sub>) was followed by the method of non-isothermal kinetic anal. In the 1st step of the decomposition 2 moles of NH<sub>3</sub> are released and in the 2nd reaction step γ-Cu(C<sub>2</sub>O<sub>4</sub>)(NH<sub>3</sub>)<sub>2</sub> is formed (activation energies = 20 ± 1 and 24 ± kcal mole<sup>-1</sup>, resp.). The structures of [Cu(NH<sub>3</sub>)<sub>5</sub>](C<sub>2</sub>O<sub>4</sub>) and of γ-Cu(C<sub>2</sub>O<sub>4</sub>)(NH<sub>3</sub>)<sub>2</sub> are discussed from their ir and EPR spectra.

L5 ANSWER 86 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1973:519868 CAPLUS

DN 79:119868

TI Magnetic exchange interactions in transition metal dimers. II. Copper and nickel di- $\mu$ -azido and  $\mu$ -oxalato complexes

AU Duggan, D. Michael; Hendrickson, David N.

CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA

SO Inorganic Chemistry (1973), 12(10), 2422-31

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Variable temperature (4.2-283°K) magnetic susceptibilities were measured for  $[M_2(tren)_2(N_3)_2][B(C_6H_5)_4]_2$ , where M = Ni(II) and Cu(II), and tren is 4-(2-aminoethyl)diethylenetriamine. A relatively strong antiferromagnetic interaction ( $J = -35 \text{ cm}^{-1}$ ) was noted for the Ni dimer, whereas the magnetic susceptibility of the Cu complex exhibits no indications of interaction. The observation of a  $\Delta M_s = \pm 2$  transition in the ESR spectrum of the Cu compound indicates it to be dimeric in the solid state. Magnetic susceptibilities (4.2-283°K) were also determined for 2  $\mu$ -oxalato-Cu dimers. No exchange interactions were detected, in contrast to that ( $J = -17 \text{ cm}^{-1}$ ) observed for the  $\mu$ -oxalato-bridged Ni complexes. Differences in magnetic exchange between the Cu and Ni systems are discussed.

L5 ANSWER 87 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1973:519332 CAPLUS

DN 79:119332

TI Crystal and molecular structures of  $\mu$ -oxalato-bis[bis(ethylenediamine)nickel(II) dinitrate,  $\mu$ -oxalato-bis[[bis(2-aminoethyl)amine]copper(II)] diperchlorate, and  $\mu$ -oxalato-bis[[bis(3-aminopropyl)amine]zinc(II)] diperchlorate

AU Curtis, Neil F.; McCormick, I. Ross N.; Waters, T. Neil

CS Chem. Dep., Victoria Univ., Wellington, N. Z.

SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1973), (15), 1537-48

CODEN: JCDBTI; ISSN: 0300-9246

DT Journal

LA English

AB The crystal and mol. structures of  $C_{20}H_{16}N_4O_{12}[Ni(en)_2]_2(NO_3)_2$  (I),  $(C_{20}H_{16}N_4O_{12})[Cu(C_4H_{13}N_3)]_2(ClO_4)_2$  (II), and  $(C_{20}H_{16}N_4O_{12})[Zn(C_6H_{17}N_3)]_2(ClO_4)_2$  (III) were determined from x-ray photog. data by the heavy atom method and refined by least squares to R 0.105, 0.101, and 0.090, for 2226, 2400, and 1195 independent reflections, resp. Crystals of I are monoclinic, space group  $P2_1/n$ , with  $Z = 2$ ,  $a$  6.33,  $b$  12.03,  $c$  14.95 Å, and  $\beta$  91.2°. Crystals of II are orthorhombic, space group  $Pnc2_1$ , with  $Z = 4$ ,  $a$  7.02,  $b$  13.25, and  $c$  25.27 Å. Crystals of III are orthorhombic, space group  $Pna2_1$ , with  $Z = 4$ ,  $a$  13.38,  $b$  14.72, and  $c$  13.30 Å. The complex cations in I, II, and III are dimeric with the planar  $C_{20}H_{16}N_4O_{12}$  group acting as a bridge by forming 5-membered chelate rings with 2 metal atoms. Coordination geometries are approx. octahedral in I, square pyramidal in II with oxalate O atoms occupying 1 basal and 1 axial site, and trigonal bipyramidal in III with oxalate O atoms occupying 1 apical and 1 equatorial site. The conformations of the ligand amines are discussed and their relations with the metal stereochem. and with the H-bonding network are examined

L5 ANSWER 88 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:490776 CAPLUS

DN 69:90776

TI Isomerism of oxalatodiamminecopper(II) complex

AU Garaj, J.

CS Slovak Tech. Univ., Bratislava, Czech.

SO Chemical Communications (London) (1968), No. 15, 904-5

CODEN: CCOMA8; ISSN: 0009-241X

DT Journal

LA English

AB X-ray diffraction studies indicate that  $\alpha$ - $Cu(NH_3)_2C_{20}H_{16}N_4O_{12}$  (which was crystallized from aqueous solns.) has orthorhombic symmetry, space group  $Pn2_1a$ ,

with unit cell dimensions  $a = 6.421$ ,  $b = 7.241$ ,  $c = 11.488$  Å., volume;  $d$ . (exptl.) = 1.96,  $Z = 4$ , and  $d$ . (calculated) = 1.97. Coordination about the Cu is approx. octahedral. Two of the trans-O bonds are considerably longer than the other 4 bonds and are unequal. The planar C2O4<sup>2-</sup> form bridges between the Cu(II) polyhedra. Single crystals of  $\beta$ -Cu(NH<sub>3</sub>)<sub>2</sub>C<sub>2</sub>O<sub>4</sub> were not obtained. X-ray diffraction studies of the dihydrate indicate that the  $\beta$ -form has a compressed octahedral ligand configuration with 2 shorter Cu-N bonds and 2 pairs of longer Cu-O bonds. NH<sub>3</sub> ligands are trans in both forms. The difference between the 2 forms lies in the functions of the C<sub>2</sub>O<sub>4</sub><sup>2-</sup> group in the structures and in the detailed configurations of the Cu(II) atoms. Diagrams of both forms are given.

L5 ANSWER 89 OF 89 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:448832 CAPLUS

DN 69:48832

TI Some oxalato-amine complexes of nickel(II), copper(II), and zinc(II)

AU Curtis, N. F.

CS Victoria Univ. Wellington, Wellington, N. Z.

SO Journal of the Chemical Society [Section] A: Inorganic, Physical, Theoretical (1968), (7), 1584-7

CODEN: JCSIAP; ISSN: 0022-4944

DT Journal

LA English

AB Preps. of the compds. [ $\text{Ni}(1,3\text{-pn})_2\text{C}_2\text{O}_4$ ](ClO<sub>4</sub>)<sub>2</sub>·H<sub>2</sub>O, [ $\text{Ni}(\text{dpt})\text{H}_2\text{O}$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, [ $\text{Cu}(\text{dien})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> (and hydrate), [ $\text{Cu}(\text{dpt})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, [ $\text{Zn}(\text{en})_2$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, [ $\text{Zn}(\text{dpt})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, and [ $\text{Zn}(\text{trien})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, considered to have dimeric structures with bridging bichelate oxalate ions, are described. The pairs of compds. [ $\text{M}(\text{en})_2$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> and [ $\text{M}(\text{trien})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> [M = Ni(II) or Zn(II)] are isostructural, whereas the pair [ $\text{M}(\text{dpt})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub> [M = Cu(II) or Zn(II)] are not isostructural. The racemic isomer of the cyclic tetramine 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane forms an analogous compound, [ $\text{Ni}(\text{tet b})$ ]<sub>2</sub>C<sub>2</sub>O<sub>4</sub>](ClO<sub>4</sub>)<sub>2</sub>, whereas the mesoisomer forms only a simple oxalate, Ni(tet a)<sub>2</sub>C<sub>2</sub>O<sub>4</sub>, and its trihydrate, considered to have polymeric structures with bridging, bi-unidentate oxalate ions. The compds. [ $\text{Zn}(1,3\text{-pn})_2$ ](ClO<sub>4</sub>)<sub>2</sub> and [ $\text{Zn}_3(\text{trien})_4$ ](ClO<sub>4</sub>)<sub>6</sub> were also prepared. The ir spectra and magnetic susceptibilities ( $\mu_{\text{eff}}$  .apprx.3 Bohr magnetons (B.M.) for the Ni compounds and .apprx.1.8 B.M. for the Cu compds.) are reported [1,3-pn = 1,3-diaminopropane: dien = diethylenetriamine: dpt = dipropylenetriamine: trien = triethylenetetramine).